

Science & Technology

REVIEW

July/August 2008

National Nuclear
Security Administration's
Lawrence Livermore
National Laboratory

Moving Technologies to Market

Also in this issue:

- **Embedded Sensors for Stockpile Stewardship**
- **A Grand Simulation of a Nanoparticle**
- **Safeguarding Nuclear Reactors**

About the Cover

Partnering with private industry can provide expertise that researchers at Lawrence Livermore need to accomplish the Laboratory's missions. At the same time, companies that license and commercialize Livermore technologies have an opportunity to achieve great success. The Industrial Partnerships Office (IPO) is Livermore's primary connection to the private sector and the conduit through which innovative inventions are transferred to commercial firms. The article beginning on p. 4 describes new efforts by the IPO staff to increase licensing agreements and make Laboratory technologies more attractive to external collaborators. The cover shows a test stand for ion-source development, a component of the proton accelerator now licensed to TomoTherapy, Inc., for cancer therapy.



Cover design: Daniel Moore

About the Review

At Lawrence Livermore National Laboratory, we focus science and technology on ensuring our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published six times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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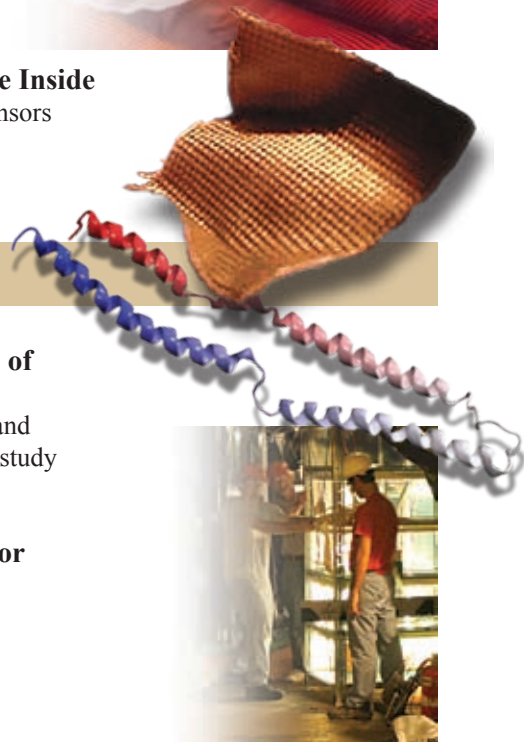
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Two planets found in nearby solar system

A team of international scientists, including three Livermore researchers, discovered a solar system nearly 5,000 light years away that contains two scaled-down gas giant planets. The two planets are the same distance apart as Jupiter and Saturn are from each other, but they are only half the distance from their parent star as Jupiter and Saturn are from our Sun. "It looks more like our solar system than any other system we've seen so far," says Livermore scientist Bruce Macintosh, "and it has room for a planet like Earth."

The Optical Gravitational Lensing Experiment detected the first evidence of these planets in 2006 when the star orbited by the planets crossed in front of a star farther from Earth, producing an effect called gravitational microlensing. In a microlensing event, the nearer star's gravity magnifies the light shining from the farther star. The planets' orbits of their parent star altered this magnification in a distinctive pattern. After the initial microlensing discovery, astronomers working at ground-based telescopes around the world observed the event and helped analyze the data. Results from the team's research appeared in the February 15, 2008, issue of *Science*.

The two new planets have mass and separation ratios and equilibrium temperatures similar to those of Jupiter and Saturn. Their masses are about 71 percent of Jupiter's mass and 90 percent of Saturn's. Their parent star is about 50 percent the mass of our Sun. This exoplanetary system, the fifth to be detected via microlensing, indicates that the Milky Way Galaxy is home to many solar systems like ours.

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Study reveals seismic structure of deep Earth

Livermore scientists and collaborators from the University of Washington, the Carnegie Institution of Washington, and Northwestern University are working to better understand the seismic structure of deep Earth by examining the elastic behavior of iron-containing minerals under extremely high pressures. The researchers have determined for the first time the complete elasticity of ferropericlase, an iron magnesium oxide found in Earth's lower mantle, through the high-spin to low-spin electronic transition induced by high pressures.

The lower mantle composes more than half of Earth's volume and is subject to extremely high pressures and temperatures. Pressure directly affects the electronic configuration of iron in mantle minerals, such as ferropericlase. Iron exists in the high-spin state at low pressure but changes dramatically to the low-spin state under extreme pressure. The team found that this transition causes ferropericlase to soften when pressures range from 40 to

60 gigapascals. Research results were published in the January 25, 2008, edition of *Science*.

According to team lead Jonathan Crowhurst of the Laboratory's Chemistry, Materials, Earth, and Life Sciences Directorate, the lower mantle profoundly influences many terrestrial phenomena, including some that are directly relevant to Earth's inhabitants. Characterizing the physical properties of the lower mantle will allow researchers to test and refine geophysical models. "Knowledge of this deep, inaccessible region is derived largely from seismic data," says Crowhurst. "It is particularly desirable to measure under relevant conditions the acoustic characteristics of candidate materials or mixtures."

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Rapid diagnosis of foot-and-mouth disease

In collaboration with the University of California at Davis, Livermore researchers have developed a rapid test to diagnose foot-and-mouth disease and other look-alike animal diseases. The prototype tool combines assays for seven disease-causing viruses into one test that simultaneously analyzes genetic material from RNA and DNA viruses. The team's results were published in the March 2008 issue of the *Journal of Clinical Microbiology*.

Researchers at the Institute for Animal Health's Pirbright Laboratory in the United Kingdom tested the prototype using 287 samples collected from cattle suspected of having foot-and-mouth disease. Assays used in the diagnostic included several previously defined viral signatures as well as new signatures identified by KPATH, Livermore's bioinformatics software system. In initial tests, the multiplex assay had a diagnostic sensitivity to foot-and-mouth disease of 93.9 percent, which is close to the 98.1 percent achieved when just two single assays are combined. Work is under way to optimize the tool's performance. Because it tests for multiple viruses in one reaction, the diagnostic will not only reduce the use of reagents and other resources but also increase confidence in test results.

According to Livermore chemist Ben Hindson, who leads the research team, assay development is in the early stages. Extensive validation tests will be required before the technology can be used routinely. The researchers are also developing assays to detect species-specific swine or cattle diseases.

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Nanotweezers save time and energy

A collaboration involving scientists from Lawrence Livermore and Lawrence Berkeley national laboratories and the University of California campuses at Berkeley and Los Angeles used nanometer-scale optoelectronic tweezers to manipulate individual

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Science Translated for the Greater Good

ALMOST all of us have been touched in some way by the ravages of cancer. My family is no exception, which makes me thrilled—and humbled—to be part of an organization that is helping make cancer treatment more effective. I know from first-hand experience that surgery, chemotherapy, and radiation are highly unpleasant procedures; yet, they succeed in saving more lives than ever before. Lawrence Livermore's new proton accelerator may be the best method yet for treating certain kinds of tumors buried deep inside the body. Where other forms of radiation damage healthy tissue before zapping the tumor, proton radiation produces far less collateral damage. Until now, proton therapy systems have weighed hundreds of tons, occupied the space of a basketball court, and required a hefty dollar investment. Remarkably, the technology embodied in a small, inexpensive accelerator developed at the request of the Department of Energy (DOE) in support of weapons research may revolutionize cancer treatment.

Translating national security research and development into better health may seem odd. Yet, translations such as this one—to new medical devices, improved manufacturing processes, new research tools, and other applications—occur often at Livermore. I have been struck by the extraordinary ability of our scientists and engineers to think about problems in new ways and to adapt an invention designed for one use to an entirely different application.

The Industrial Partnerships Office (IPO), described in the article beginning on p. 4, is the Laboratory's primary link to the private sector and real-world users of our inventions. As such, IPO plays a pivotal role in making any translation succeed. The staff of IPO and its predecessor organization, the Industrial Partnerships and Commercialization Office, are experts at forging relationships with companies eager to commercialize Livermore's latest developments. For example, an IPO business development executive found a partner to commercialize the proton accelerator to treat cancer. A firm that specializes in innovative radiation treatments, TomoTherapy, Inc., has made a significant investment in the collaborative development of a marketable prototype.

IPO plays an important role in helping to increase the work that Livermore does with new sponsors. Funding from our traditional DOE sponsors declined for fiscal year 2008, which means that funding for the Laboratory Directed Research and Development Program, our primary tool for advancing basic science, has also declined. More cooperative agreements such as the one with TomoTherapy will help keep Laboratory research on the cutting edge.

IPO Director Erik Stenehjelm and his staff are also working aggressively and creatively to increase the number of Laboratory inventions that are commercialized by private firms. Royalties from commercial licenses feed our translational abilities by allowing us to invest that much more in basic science and technology developments. Stenehjelm's team is making excellent use of resources outside the Laboratory to attract venture capital and commercial interest. For example, IPO is working with entrepreneurial graduate students at nearby business schools to improve its marketing of new Laboratory inventions—for residential solar power, water purification, optical devices, and more. The students write business plans for real technologies and may win one of many highly remunerative business-plan competitions. IPO garners business plans that give investors and potential commercial partners everything they need to know about taking a product to market successfully.


Since joining the Laboratory in 2007, I am continually impressed with Livermore's ability to deliver exceptional science and technology. Equally impressive is IPO's track record of translating researchers' results into marketable products and processes that can improve our lives.

■ Steven D. Liedle is deputy director of Lawrence Livermore National Laboratory.

The New Face of Industrial Partnerships

Livermore's Industrial Partnerships Office has a new name, a new director, and ambitious new goals.

Livermore's Industrial Partnerships Office (IPO) helps the Laboratory transfer innovative inventions to the private sector. For example, laser peening (above), a spin-off technology from Livermore's laser research, can be used to increase the strength of welds in critical metal parts. (Image courtesy of Metal Improvement Company.)



THE director of Livermore's Industrial Partnerships Office (IPO) posted a brief notice one day last March for a series of lectures he planned to give in April on "Developing Business Models for Emerging Technologies." Attendance was to be limited to 30 individuals. Forty people inquired within a day, and 60 scientists, engineers, and other employees from across the Laboratory came to listen and learn.

Lawrence Livermore has been a leader for many years among Department of

Energy (DOE) laboratories in licensing and commercializing the technologies it develops. But IPO Director Erik Stenehjem (pronounced sten-yem) and his staff have big plans to significantly expand business activities with private firms and nonfederal entities, including doubling over the next five years the number of commercial licenses.

Stenehjem came to Livermore from Pacific Northwest National Laboratory and its managing organization Battelle as part

of the public-private consortium that now operates Lawrence Livermore National Laboratory. (See the box on p. 10.) At Pacific Northwest, Stenehjem managed new ventures and regional initiatives. Battelle is a national leader in commercializing technologies.

Stenehjem has only good things to say about the staff at IPO (formerly called Industrial Partnerships and Commercialization). Among the seven business development executives and the

management team, six individuals have a Ph.D. in science or engineering, five are attorneys, three have experience in startup companies, and four are registered patent attorneys. Some staff members wear more than one of these hats. Over the last several years, the capable staff has successfully commercialized dozens of Livermore technologies for homeland security, health care, manufacturing, and more. "It's a highly talented group," says Stenehjem. "Last year, they returned more than \$6 million in royalties to the Laboratory. Combined with the industry funding from cooperative agreements, that yielded almost \$3 for every dollar spent by the office."

Why Partner?

Since the Laboratory's founding in 1952, its mission has been to ensure national

security and find science and technology solutions to our nation's problems. Partnering with industry brings the additional expertise needed to accomplish the Laboratory's mission. At the same time, many private companies that have licensed and commercialized Livermore technologies are achieving great success.

Supercomputing is an excellent example of how collaborations with industry have served Livermore's goals. To model the behavior of nuclear weapon materials and components in computer simulations, Livermore researchers have created a virtually insatiable demand for computing power. That demand drove the design of the first supercomputers and led to partnerships with IBM, Control Data Corporation, and Cray, among many others. Under the National Nuclear

Security Administration's Advanced Simulation and Computing Program, partnerships with IBM have led to the development of many breakthrough machines, including the Blue Gene line of supercomputers. BlueGene/L, Livermore's largest computing resource, is helping researchers perform both classified and unclassified research.

Collaborations with private industry have also been crucial in developing the Laboratory's record-shattering lasers over the last four decades. For the National Ignition Facility, the world's largest laser, Livermore scientists and dozens of private firms came together to develop new tools, materials, and manufacturing methods. Many of the components in the laser system represent significant advancements of current technologies,

The IPO staff is key to Lawrence Livermore successfully licensing and commercializing its technologies.



while other components are entirely new. Commissioning of the giant laser will be complete in 2009, and experiments to achieve fusion ignition will begin in 2010.

Meanwhile, dozens of Livermore innovations have moved to the private sector. One is a laser process to strengthen metal components, making them better able to resist fatigue and corrosion. Metal Improvement Company (MIC) of Paramus, New Jersey, a firm specializing in metal treatments, licensed this Laboratory invention and continues to refine the process. Robotic laser peening is now routinely used to strengthen and form critical components of aircraft engines for longer life. MIC recently received a contract to establish a laser-peening production cell inside Boeing Corporation's Frederickson, Washington, facility. MIC's innovations also improve fatigue lifetime for components of the Apache and Blackhawk helicopters, the M1A1 Abrams tank, the F-22 fighter jet, and the B-52 bomber.

For the Laboratory's mission in homeland and global security, success depends on commercializing inventions and getting a usable product, such as a new radiation or biological-agent detector, into the hands of end users as quickly as possible. Transferring Livermore-developed technologies to the private sector makes these advances available to those who secure our borders and airports, monitor public places for biological or chemical attacks, and respond to emergencies. Working directly with private organizations helps speed the delivery of new inventions to users. IPO plays an important role in identifying and wooing industrial partners as well as in simplifying the process by which the Laboratory works with other entities. "We're exploring ways to make the contracting process faster and easier," says Stenehjem.

One technology important for homeland security is an ultrawideband (UWB) device that can monitor cargo containers and detect unauthorized entry. Every year,

Collaborations with private industry have been important for the National Ignition Facility (NIF). For example, NIF worked with Hoya Corporation and Schott Glass Technologies, Inc., to develop a production method that continuously melts and pours the glass needed to amplify the laser light for experiments. Shown here, an employee at Hoya inspects a sheet of glass as it moves down the assembly line.



A partnership between Livermore and IBM led to the development of BlueGene/L, one of the most capable computing machine in the world. The unusual slant to the BlueGene/L cabinets is a necessary design element to keep cooled air flowing properly around each cabinet's 2,000-plus processors.

more than 200 million shipments transport 90 percent of the world's cargo on trains, airplanes, ships, and trucks. Concern about a terrorist organization using a cargo container to deliver a weapon of mass destruction into the U.S. led to the development of an inexpensive, reliable, and reusable detection device called SecureBox.

The device uses UWB technology first developed at Livermore in the early 1990s with funding from the Laboratory Directed Research and Development (LDRD) Program. Modern UWB technology at Livermore uses coherent, broad-spectrum, low-power pulses, which allow devices to be highly sensitive to intrusions into a preset area of coverage while consuming considerably less power than a narrowband device with comparable sensitivity. The SecureBox UWB device can detect an intrusion through any of a container's six walls, whether it be from a door opening or from a cut through a container wall. It can then send an alarm to authorized individuals.

The Secure Box Corporation of Santa Clara, California, licensed the technology and subsequently invested \$500,000 in a Cooperative Research and Development Agreement (CRADA) with Livermore to customize the core technology for the cargo security application and to explore uses for the SecureBox device by the U.S. government. The device's efficacy was demonstrated by the Laboratory during the 2006 Canada-U.S. Cargo Security Project, Phase 2. More recently, the technology has been tested in exercises in Europe and the San Francisco Bay Area and with the U.S. Coast Guard.

Innovation Breeds Success

Another Laboratory-inspired venture may radically improve the way cancer patients receive treatment. Last year, a private firm licensed an accelerator technology that Livermore first explored with LDRD funding to take x-ray images

deep inside nuclear weapon surrogates during nonnuclear testing. A Livermore colleague working in another program saw the accelerator concept and suspected it could be used for proton therapy, a radiation treatment that can zap tumors with a powerful, focused beam while causing minimal damage to surrounding healthy tissue. This idea led to yet another LDRD project, one that would explore the technology for building small proton accelerators that could be used in cancer radiation therapy. In 2004, the University of California (UC) Davis Cancer Center began partnering with the Laboratory on this project and matched the LDRD investment.

Radiation from traditional x- and gamma-ray treatments often damages healthy tissue as it travels on its path to the target tumor. Protons, because of their positive charge and high mass, retain most of their energy until they reach the cancer site. Many doctors consider protons to be superior to x rays for treating certain kinds of cancers. However, current proton accelerators are expensive machines that weigh several hundred tons and are the size of a basketball court. Only about half a dozen cancer treatment centers in the U.S. have systems for proton therapy. When Livermore's device is fully developed, it will be just 2 meters long and deliver the necessary beam energy at a fraction of the cost of current systems.



SecureBox is a wireless device that can be installed on cargo containers to detect intrusions.

Researchers at the UC Davis Cancer Center acted as matchmaker for licensing the accelerator technology. UC Davis had purchased another type of radiation therapy machine from TomoTherapy, Inc., of Madison, Wisconsin, a firm specializing in radiation treatment for cancer. In 2005, UC Davis invited Livermore scientists to

present their technology to TomoTherapy. In 2006, UC Davis signed a second partnership agreement with the Laboratory to further develop the accelerator for cancer therapy.

Meanwhile, IPO business development executive Genaro Mempo was negotiating with TomoTherapy and other interested companies. "After more than a year, TomoTherapy licensed the technology in February 2007," says Mempo. TomoTherapy is contributing funding to Livermore through a CRADA and now works with both UC Davis and the Laboratory to develop a prototype, which will be tested at UC Davis.

Physicist George Caporaso, who led the team that originally explored the accelerator concept for defense-related use, is thrilled to see this new application. "The idea to use the accelerator for cancer

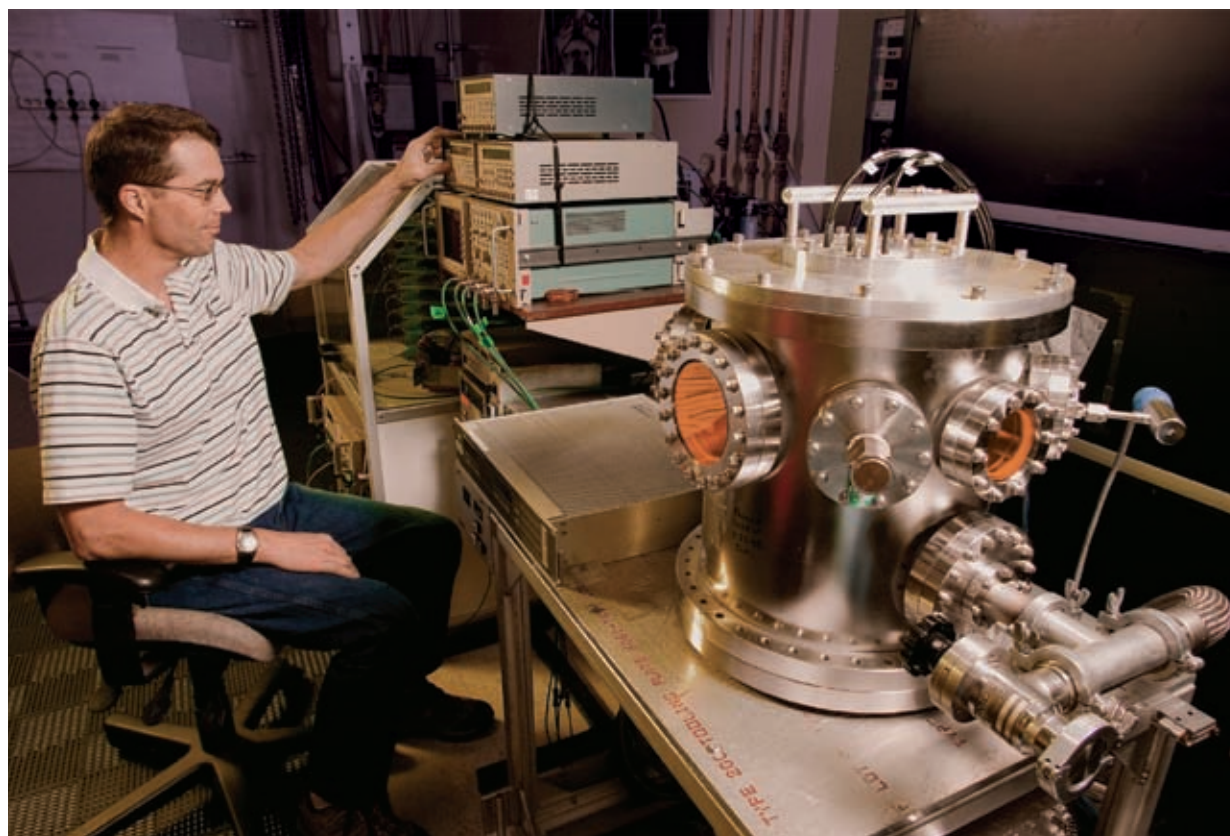
treatment came from Dennis Matthews [now at UC Davis Cancer Center]," says Caporaso. "I would never have thought of it, and it may well revolutionize cancer treatment." TomoTherapy has four employees at the Laboratory, working alongside their technical counterparts. Caporaso leads the collaboration with UC Davis and TomoTherapy.

Crossing the Valley of Death

Stenehjem and his team are taking an aggressive approach to vaulting inventions across the "Valley of Death," the funding gap that typically exists between a laboratory invention and a marketable prototype. The technologies developed at institutions such as Livermore are highly effective at doing what they are designed to do, but they may be unsuitable outside a research environment and difficult to

operate without training. Or, as with the compact accelerator, the invention may be targeted at a market totally different from that for which it was conceived. The Laboratory typically cannot pay to develop the commercial version of its invention. Yet, venture capitalists and private companies are inclined to invest only in technologies or products that are proven and ready for use.

At Livermore, every IPO business development executive keeps tabs on competing patents and other intellectual property for a particular area of Laboratory research. He or she also follows relevant markets and private companies that might be interested in a new invention. In addition, Livermore-developed technologies are posted on the *Federal Business Opportunities* Web site. However, these efforts may not be enough to attract



James Watson sets up a test stand for ion-source development, one component of the compact proton accelerator designed for cancer therapy.

either venture capital or a company to license a technology, in which case the Valley of Death looms ahead.

Livermore and UC Davis were so convinced of the potential for the small accelerator as a cancer therapy tool that the two institutions invested in it, avoiding the Valley of Death. Livermore's IPO and its counterpart at UC Davis each invested \$1.5 million to ready the technology for the marketplace, a process called technology maturation. Their continued efforts on the

device helped make it more marketable, enough so that TomoTherapy was willing to invest in the collaboration.

Business Plans Are Win-Win

One way to help leapfrog the Valley of Death to successful commercialization is to develop a solid business plan. Few funding organizations will consider investing in a new technology that does not have well-researched numbers on the technology's viability in the marketplace,

its competition, proposed company management, pricing, and details of required funding. Most Laboratory researchers are not business planning experts, so IPO is working with graduate-student scientists and engineers who are in programs on entrepreneurship at several nearby universities. These students draw up business plans for Livermore technologies.

School-sponsored competitions for student-written business plans award as much as \$250,000 to the winner. Students want to prepare a winning business plan, yet they often have to dream up a product or technology to write about. The increased prize money and popularity of the contests has led student teams to seek compelling high-tech products as subjects for their business plans. If a student writes a business plan for a Livermore technology, he or she may win the competition, and the Laboratory gets a business plan it can take to venture capitalists. Everyone wins.

Livermore has had some success in the past with student-written business plans. However, Stenehjem is being more aggressive with this tool, on the assumption that more business plans will translate into a higher number of technologies licensed by well-financed companies. Last year, Stenehjem tapped physicist Ralph Jacobs to establish an outreach program to area business schools. Jacobs has extensive laser science experience at the Laboratory and started a successful firm in California's Silicon Valley, where he worked in the 1980s. The company was purchased in 2000 for what was then the largest takeover offer for a high-tech company.

Stenehjem, Jacobs, and others sifted through more than 900 Livermore patents to find ones that represented a "disruptive" or revolutionary technology, could be commercialized in about two years, and were unencumbered by other licenses or CRADAs. "Some patents involved only

New Director of the Industrial Partnerships Office

Erik Stenehjem, with a Ph.D. in economics, brings to Livermore an impressive record of successful technology transfer and entrepreneurship. At Pacific Northwest National Laboratory (PNNL), he was responsible for creating new technology-based ventures and building partnerships with institutions in the Pacific Northwest, a job similar to his position at Livermore. At PNNL, he worked with regional research institutions, including universities in Washington and Oregon, to find and bundle technologies and pair them with economic activity within the region. PNNL is in rural southeastern Washington, far from major urban centers. He had to reach out—far out, in many instances—to take new technologies into the marketplace.

In 2006, the State of Oregon appointed Stenehjem to serve as science and technology advisor to Governor Ted Kulongoski. He also served on the Washington Economic Development Commission's steering committee for technology commercialization and the board of advisors for the University of Washington's Center for Innovation and Entrepreneurship. At both the University of Washington and Washington State University, Stenehjem taught courses on entrepreneurship and new business creation in masters in business administration programs. He led students into business plan competitions, with the goal of developing new businesses to enhance the Washington state economy.

Before joining Battelle, which manages PNNL, he founded his own business in the early 1980s. He assisted clients in forecasting and mitigating the effects of rapid economic growth and decline on regional economies. Stenehjem not only talks the talk, but on his own, he has walked the walk.



Erik Stenehjem joined the Laboratory in 2007 to lead the Industrial Partnerships Office.

an incremental change to an existing device or process,” says Jacobs, “while others were too futuristic.” Ultimately, the reviewers selected 17 standout technologies, including a residential solar thermal power plant, a method to generate electricity from waste heat, electromechanical batteries, nanolaminate capacitors, nanolaminate mirrors, and a water treatment process using carbon nanotubes.

The 17 technologies were advertised on IPO’s Web site (ipo.llnl.gov) and by Jacobs and Stenehjem during visits to classes on entrepreneurship at nearby business schools. Several business schools signed on, including UC Davis, UC Berkeley, University of San Francisco, Golden Gate University, San Jose State University, and University of the Pacific. Jacobs says, “A student at Sloan School of Management at the Massachusetts Institute of Technology found us while surfing the Web. He also developed a plan.”

Students in masters of business administration programs completed business plans for 12 Livermore technologies, and many were entered in competitions. Three made it to the finals of various contests. The outlook for funding and commercializing these technologies indeed looks bright.

Funding is the magic word. Any new business requires four ingredients: technology, management, knowledge of the market, and money. “You need the right combination of all four pieces,” says Stenehjem. “The Laboratory has the technology, and some scientists and

engineers make good managers. The students’ business plans provide the market knowledge. That leaves money.”

Livermore is developing a close relationship with venture capitalists and “angel investors,” which are consortia of wealthy individuals. For example, Laboratory technology transfer representatives have been invited to attend monthly meetings of Keiretsu Forum, the world’s largest angel investor network with 750 accredited investor members on three continents.

Having newly minted business plans in place will give Livermore a leg up with investors. “Venture capitalists judge business plan competitions,” says Stenehjem, “and they love cutting-edge technologies.”

Into the Future

Funding more commercial ventures and startup companies based on Livermore technologies will increase royalties to the Laboratory. Most licensing and royalty income is distributed back to the Laboratory directorates, with much of the remainder going to the inventors. A small amount goes to the institution for administrative costs, readying technologies for the marketplace, and other technology-transfer activities. Toward this end, Stenehjem hopes to hire more business development executives and patent attorneys and further increase patent protection and IPO’s production level.

He has broadened the responsibilities of IPO’s business development executives.

Feedback from commercial partners indicates that they are often unaware of all the Laboratory has to offer. Partners work with a principal investigator and perhaps a few more scientists and engineers, but the rest of the Laboratory remains unknown to them. Business development executives can inform partner firms of other licensing and contracting opportunities at Livermore. Also, by serving as a central point of contact for partner firms, the IPO executives can address issues and concerns before they become problems.

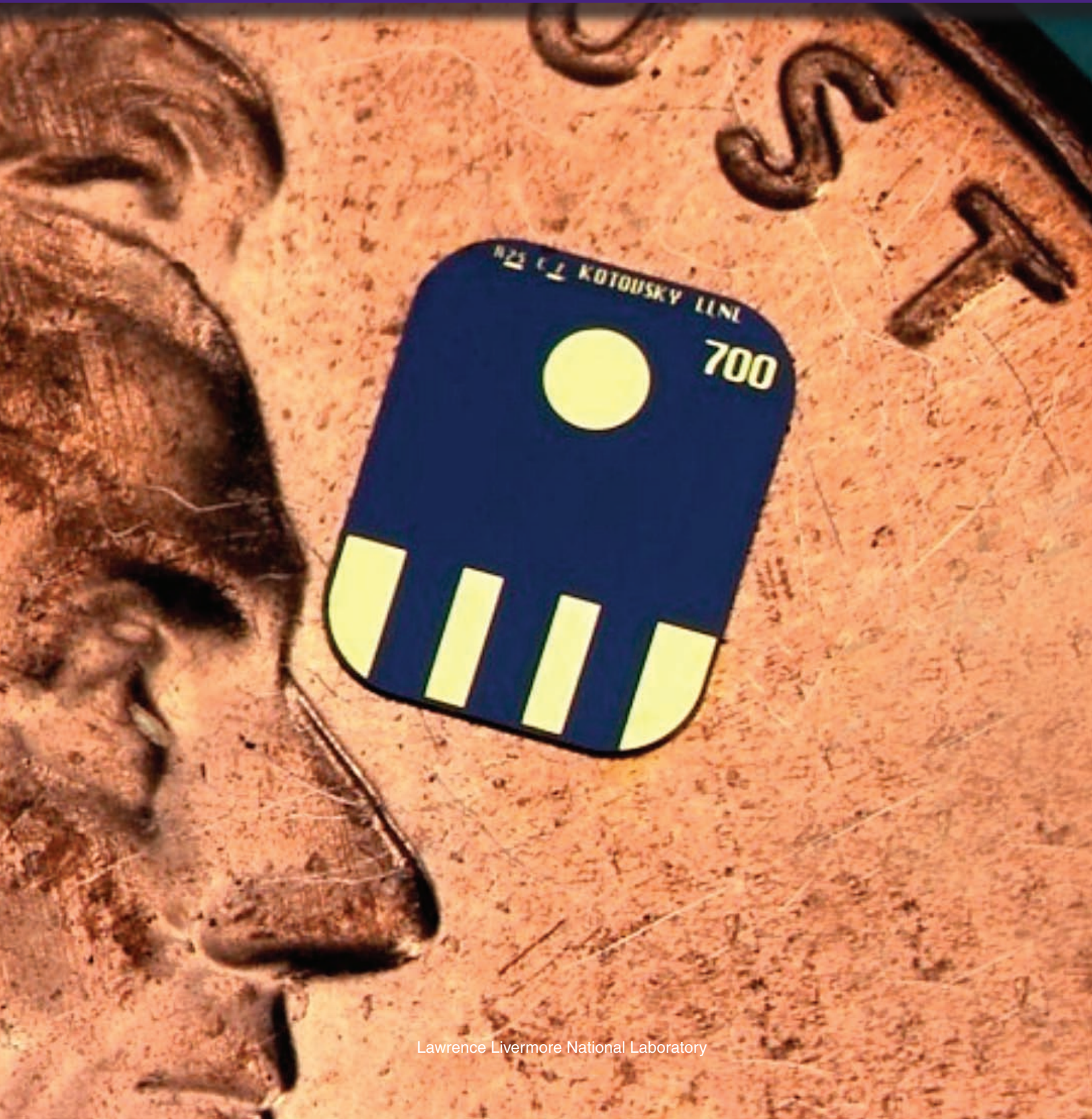
Looking further into the future, Stenehjem envisions a technology research park outside the Laboratory’s gates where scientists and engineers could more easily engage with industrial partners and develop new commercial ventures. He also hopes to explore interest in an “accelerator” that would bring together venture capitalists; serial entrepreneurs, who start a business and move on to another; market analysts; and Livermore technologies. Stenehjem’s enthusiasm is palpable. When he says, “These are exciting times,” he means it.

—Katie Walter

Key Words: commercialization, Cooperative Research and Development Agreement (CRADA), industrial partnership, laser peening, proton accelerator, SecureBox, technology transfer.

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Monitoring a Nuclear



Weapon

from the Inside

Embedded sensors could help transform stockpile stewardship.

THE paramount national security mission of Lawrence Livermore is ensuring the safety and reliability of the nation's nuclear weapons stockpile. Development of new nuclear weapons systems stopped nearly two decades ago, and today, the nation's stockpile is maintained through a science-based stockpile stewardship program. However, as weapon components age, ensuring the reliability of the stockpile has become an increasingly complicated and costly challenge.

The Department of Energy's National Nuclear Security Administration (NNSA) is working to transform the U.S. nuclear weapons complex and the nation's stockpile by shrinking the size of both and finding more cost-effective ways to maintain the remaining weapons. In short, procedures developed during the Cold War to ensure that the stockpile meets all performance requirements must be replaced with a more efficient approach, made possible by using modern technologies.

"The nuclear weapons complex is at a crossroads—maintaining the status quo is not an option we can afford," says NNSA Administrator Thomas D'Agostino. "Delay and inaction will only increase the costs and elevate the risks associated with maintaining an aging stockpile." (See the box on p. 15.)

Livermore scientists and engineers are providing technical leadership to achieve this transformation. According to Livermore physicist Jim Trebes, "Weapons are hard to maintain; we want to do the job faster, better, and cheaper." One of the most needed improvements is a cost-effective method to collect data about the state of nuclear weapon components, in particular, to detect corrosion, cracks, and composition-changing properties without having to dismantle the weapons. Traditionally, a few randomly selected warheads and bombs are pulled from the field every year and transported to NNSA's Pantex Plant in Texas, where they are disassembled for close inspection. While

Tiny sensors similar to the one shown here could be embedded in the nation's nuclear weapons to detect anomalies such as cracks or corrosion in weapon components.

most are reassembled and returned to the stockpile, at least one warhead of each type is destroyed in the process. Some parts, for example, are cut open for inspection, and others are stressed to the failure point.

A promising Livermore effort is developing tiny, rugged sensors that could be embedded in every nuclear weapon. Embedded sensors, compatible with warhead materials, could provide information currently obtained from disassembly. Such devices could make possible for the first time “persistent surveillance”—continuous monitoring of the state of health for every weapon and practically instantaneous detection of anomalies.

Eliminating the costly and sometimes destructive testing of warheads is particularly important to comply with the Moscow Treaty on Strategic Offensive Reductions, which was signed in 2002. Under the terms of this treaty, the U.S. is reducing its total number of active nuclear

weapons to between 1,700 and 2,200 warheads and bombs. As the number of U.S. weapons shrinks, fewer weapons are available for disassembly to provide statistical assurance about the stockpile’s health.

Sensors would most likely be embedded in existing weapons during a life-extension program—a rebuilding effort that significantly increases a warhead’s lifespan. Sensors could also be added to so-called shelf units stored at NNSA’s Y-12 Plant in Tennessee and at Pantex, where individual components are monitored closely for signs of aging and unexpected physical and chemical changes. In addition, if replacement warheads were developed, sensors could be integrated into the weapon assembly.

Once in place, an array of different sensors could signal the presence of unwanted gases, record stresses incurred as a warhead is moved, and detect microscopic cracks and voids. Trebes, who is helping guide Livermore sensor designs, notes that an embedded sensor network might also reveal “unknown unknowns,” issues not previously encountered.

“If we could assess every weapon in real time, we would immediately know which warheads need to be pulled apart, and that would drive down costs,” says chemist Lou Terminello, who leads the Laboratory’s

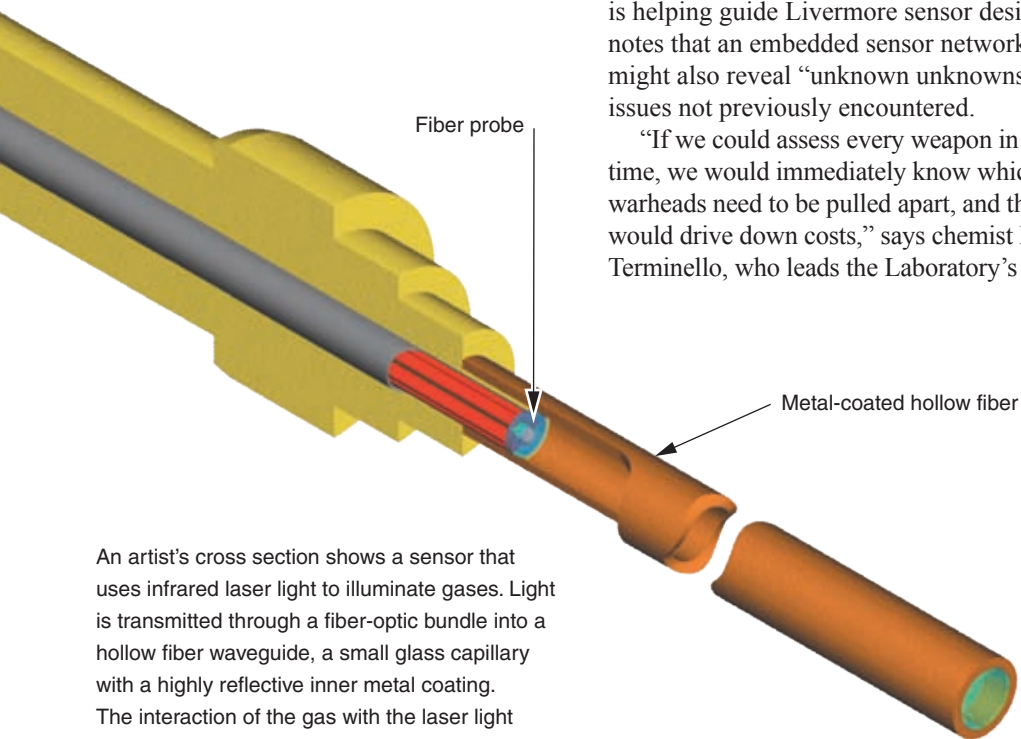
materials program. Bruce Goodwin, principal associate director for Weapons and Complex Integration, adds, “Embedded sensors have the potential for a huge payoff in costs and manpower. They will give us stronger confidence in the stockpile. Instead of sending all 30 kids in a classroom to get a physical exam, one kid raises his hand and says, ‘I’m sick.’”

Diverse Sensor Development Team

The sensor development program includes about 15 engineers, chemists, physicists, and computational scientists. The effort taps Laboratory expertise in microfabrication, forensic science, nuclear chemistry, photonics, medical technology, homeland security, and computer modeling. The developers were inspired, in part, by the electronic sensors that monitor dozens of parts and systems in cars. Experimenters at the Laboratory’s High Explosives Application Facility have also successfully used microscopic sensors for several years, embedding them in high-explosive formulations to track aging effects.

Livermore’s Laboratory Directed Research and Development Program funds much of this research through the Transformational Materials Initiative, which is focused on creating materials, processes, and diagnostics to support NNSA’s complex transformation. New technologies can also be applied to other fields, including energy, nonproliferation, global security, and health care. According to Livermore physicist Robert Maxwell, who leads this research effort, “The initiative has allowed us to pursue advanced sensor ideas.” Designs that mature beyond the proof-of-principle stage are then funded by NNSA.

Collaborating institutions include Georgia Institute of Technology, University of South Carolina, the United Kingdom’s Atomic Weapons Establishment (AWE), and other NNSA sites. A joint working group, with representatives from throughout



An artist's cross section shows a sensor that uses infrared laser light to illuminate gases. Light is transmitted through a fiber-optic bundle into a hollow fiber waveguide, a small glass capillary with a highly reflective inner metal coating. The interaction of the gas with the laser light identifies the gas.

the NNSA complex, holds a monthly teleconference to discuss issues and monitor sensor development. “We want to leverage the capabilities of our partners,” says engineer Tony Lavietes, who leads the Laboratory’s microsensors program. In addition, an annual workshop is held at Livermore, with more than 100 people from the U.S. and AWE in attendance.

Trebes describes the ideal weapon sensor as a device with zero size and weight. Measuring a few millimeters in diameter and weighing a few milligrams, Livermore sensor designs nearly reach that impossible standard. The biggest obstacle, however, is durability. Industry typically builds sensors to last a few years, but in weapons, sensor lifetimes must be 10 times longer. Once embedded, sensors cannot be easily accessed for



This prototype of a Livermore-designed sensor uses 20 glass fibers, each 300 micrometers in diameter, surrounding a fiber in which laser light illuminates gas contained in a glass capillary. The center fiber is 420 micrometers in diameter.

Transforming the Nation’s Nuclear Stockpile

When the U.S. stopped nuclear testing in 1992, scientists and engineers at the Department of Energy (DOE) nuclear weapons laboratories embarked on a vigorous effort to acquire the tools for a science- and technology-based stockpile stewardship program. This program includes advanced computing, high-energy-density physics, experimental capabilities, modern diagnostics facilities, and enhanced surveillance techniques. Together, the tools provide the data needed to predict how aging will affect warheads and ensure that the stockpile continues to meet all performance requirements. In this way, components can be replaced before they degrade overall system reliability and safety.

According to Thomas D’Agostino, administrator of the DOE’s National Nuclear Security Administration, “Today’s stockpile remains safe, reliable, and does not require nuclear testing. This assessment is based on a foundation of past nuclear tests, scientific and engineering experiments and analysis including improved warhead surveillance, and the independent judgment of Lawrence Livermore and Los Alamos directors advised by their weapons program staffs.”

Livermore scientists and engineers have long conducted research for assessing the safety, security, and reliability of weapon designs and for annually certifying the nation’s stockpile. In recent years, the emphasis has turned to developing methods to accomplish those activities with a smaller, safer, and more cost-effective nuclear weapons complex. Livermore’s program to design embedded sensors that would promptly indicate problems in warheads is one example of the new focus on transforming the nuclear weapons complex and the stockpile.

Rethinking stockpile stewardship has assumed increased urgency as the number of warheads and bombs shrinks. In 2002, U.S. President George W. Bush and Russian President Vladimir Putin signed the Moscow Treaty on Strategic Offensive Reductions. To comply with this treaty, the U.S. must reduce the number of operationally deployed strategic nuclear warheads to between 1,700 and 2,200 by 2012. In 2004, President Bush issued a directive to cut the entire U.S. nuclear stockpile—both deployed and reserve warheads—in half by 2012. This goal was achieved in 2007, five years ahead of schedule, making the total stockpile almost 50 percent less than it had been in 2001.

President Bush has proposed reducing the stockpile another 15 percent, less than one-quarter its size at the end of the Cold War. To ensure that such a reduced stockpile—the smallest in more than 50 years—would address specific threats, Congress has directed DOE to work with other federal agencies on a comprehensive review of the nation’s nuclear strategy for the 21st century.

repair or replacement. “The supreme challenge is making a sensor remain reliable and robust for 40 years,” says Trebes. “There is no reason to put sensors in warheads if we are not confident they will continue to function for decades.”

An exhaustive qualification process will ensure that sensors can operate in the hostile environments deep within a nuclear warhead. Livermore and AWE researchers are conducting centrifuge tests on some prototypes, and extreme environmental tests, including hydrodynamic experiments at Livermore’s experimental test site, will be scheduled.

Laboratory researchers are also devising methods to extract data from the sensors. One concept is to develop a portable diagnostics unit that will download sensor data and provide the necessary power sources, lasers, and data-acquisition hardware. A military technician would then

attach the diagnostics unit to a deployed warhead, in much the same way that a technician plugs a cable into a port in a car to assess the status of engine components. Separating the embedded sensors from power sources, data-acquisition devices, and lasers ensures optimum safety and reduces the potential for obsolescence.

Optical Fibers in Sensors

Many sensor designs use glass fibers measuring about 75 micrometers in diameter, smaller than the thickness of human hair. Because they have no electrical requirements, optical sensors are intrinsically safe and are ideal for use in environments that include energetic materials.

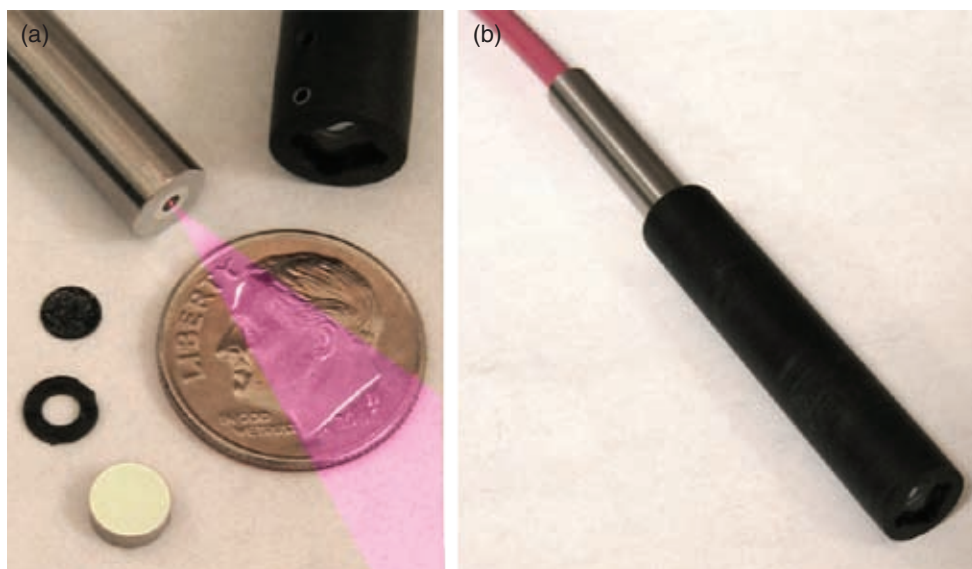
Biophysicist James Chan is working with colleague Chance Carter on a gas sensor that can measure material degradation at a parts-per-million level

of concentration. “We’re developing optical methods to monitor chemical processes that produce any type of outgassing,” says Chan. “If we catch outgassing at an early stage, we can identify which material is decomposing or corroding and mitigate the problem quickly.” The Livermore scientists are collaborating with professors Boris Mizaikoff of the Georgia Institute of Technology and Mike Angel of the University of South Carolina and their graduate students.

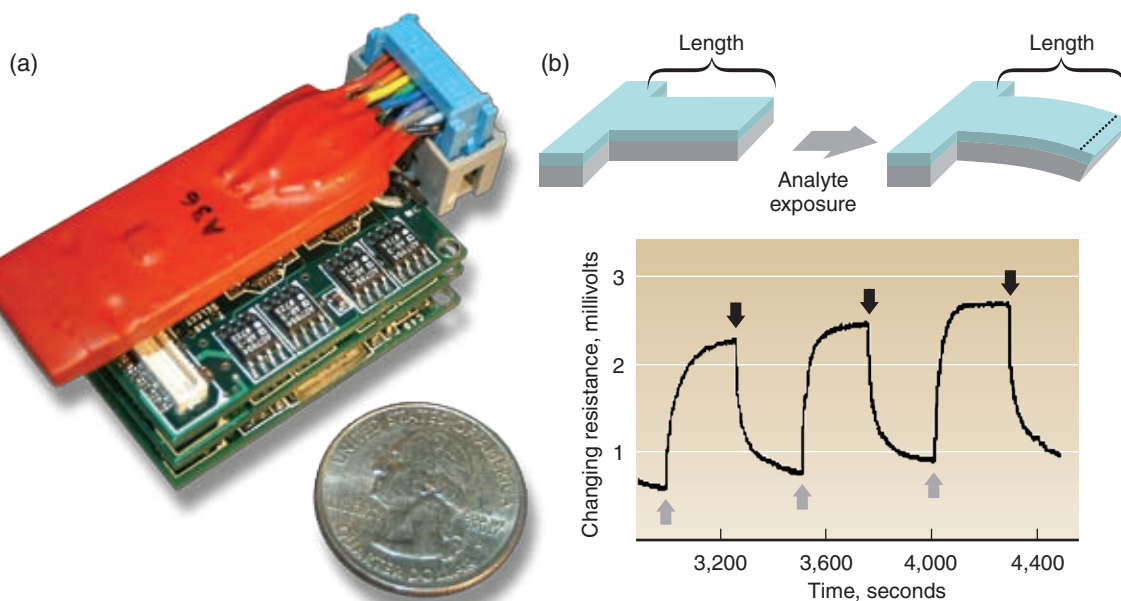
Chan notes that gas sensors are common in manufacturing plants, environmental monitoring systems, and vehicles. Most of these sensors, however, target just one or a few compounds. A major challenge for the Livermore team is to build a sensor that detects a range of volatile compounds.

The team developed prototypes that use Raman and infrared spectroscopy as complementary techniques to identify gases. Both techniques measure the response of molecular bonds to a beam of infrared light generated by a laser and sent through a fiber optic into a hollow fiber waveguide, a small glass capillary with a highly reflective inner metal coating. Infrared spectroscopy measures the amount of light absorbed, which yields a “fingerprint” of the gas. In contrast, Raman spectroscopy records the degree of light scattered by a compound, which also gives a distinct molecular fingerprint. In laboratory tests, the prototypes have accurately detected several common gases. Planned experiments will test for a wider range of gases.

Livermore biophysicist Ward Small is developing another fiber-based gas sensor, in this case to detect and capture hydrogen. This sensor uses a type of getter that is common in industrial applications to remove traces of explosive gases. Hydrogen is both explosive and corrosive, so hydrogen getters are required in environments such as fuel delivery systems.



(a) The components used for Livermore’s getter-based hydrogen sensor include (counterclockwise from top) the sensor case; a fiber bundle, consisting of a central laser delivery fiber surrounded by six light-collection fibers; a getter made of 1,4-bis(phenylethynyl)benzene (DEB) and silicone rubber; a spacer ring; and a mirror. (b) In the assembled prototype, laser light exiting the central fiber passes through the DEB–silicone composite, reflects off the mirror, and makes a second pass through the composite before entering the collection fibers.



(a) One Livermore design uses arrays of microscopic cantilevers to detect a range of gas species. Each green board under the red connector assembly has more than one of these tiny "diving boards," which are coated with polymers a few hundred nanometers thick. (b) As shown in the artist's sketch, the polymer swells as it absorbs gas molecules, bending the microcantilever and changing electrical resistivity (voltage), thereby signaling that gas is present. The graph shows the change in resistance when a gas is introduced three times (gray arrows) and purged (black arrows).

Small is experimenting with an organic getter made of 1,4-bis(phenylethynyl) benzene, or DEB. His design uses photoacoustic Fourier transform infrared (FTIR) spectroscopy to detect changes in the physical properties of the getter, in particular, changes in the optical properties as the getter captures hydrogen. At particular wavelengths, FTIR spectroscopy shows characteristic peaks whose intensities change as DEB bonds with hydrogen atoms.

"The light must interact with the getter at the point where it captures hydrogen to maximize the sensor's sensitivity," says Small. "For example, if the light is confined to the getter surface, the sensor will not respond to changes occurring at a deeper level." FTIR spectroscopy showed that infrared light cannot pass through a getter made of pure DEB. To enable full-thickness light penetration, Small made a 125-micrometer-thick composite of silicone rubber with DEB dispersed throughout. When hydrogen molecules bond to the composite, less light is absorbed. Once embedded in a warhead, the sensor would be fed by infrared laser light supplied through an optical fiber located outside the warhead.

Small, a biomedical optics expert, is also working with light-activated shape memory polymers for treating brain aneurysms. (See *S&TR*, May/June 2008, pp. 4–12.) He notes that the two research areas have similar challenges. Chan is involved in medical research, too. He works part-time at the University of California at Davis developing diagnostic tools that use Raman spectroscopy to detect cancer.

Microscopic Diving Boards

Another kind of sensor takes a different route to detecting and measuring gas molecules, including volatile organic compounds and water vapor, both of which can indicate degradation of a component. The microelectromechanical systems (MEMS) device uses an array of what biophysicist Tim Ratto describes as microscopic silicon diving boards, each measuring about 120 micrometers long, 50 micrometers wide, and 0.5 micrometers thick.

The diving boards, also called microcantilevers, are coated with polymers a few hundred nanometers thick. The polymer swells as it absorbs gas molecules, in the process bending

the diving board. This bending changes the electrical resistivity of the cantilever, thereby signaling the presence of a gas. By measuring the pattern of deflection across an array of cantilevers, scientists can obtain the chemical signatures for a number of gases. "Our sensor reacts in similar fashion to how odorants bind to different receptors in a mammalian nose," says Ratto.

The sensor is an offshoot of a compact, low-power device that Ratto built with Livermore chemists Brad Hart and Albert Loui to detect vapor from chemical nerve and blister agents such as VX and sulfur mustard. The diving-board sensor will complement others under development, not replace them. To evaluate the design, Ratto has embedded a prototype in a test canister that serves as a simulated weapon. The microcantilever technology should also prove useful in applications such as airport explosives sniffers, food spoilage indicators, and chemical plant monitors.

Silicon Makes It Work

Livermore mechanical engineer Jack Kotovsky is developing several MEMS-based sensors, which are fabricated from silicon with techniques similar to those

used by the electronics industry. With a background in biomechanics, Kotovsky is expert at designing and building microstructures. His original MEMS contact sensor design was an offshoot of a device he developed for measuring loads on human knees.

MEMS-based sensors are ideal for use in warheads because of their small dimensions, material properties, low power consumption, and mass manufacturability. Embedded sensors must fit into spaces not originally designed to accommodate them. As a result, they must be extremely thin (about one-half the thickness of a human hair) and be able to bend, flex, and stretch to conform to any curved surface. Silicon is used as the sensor substrate because it is inert and deflects and springs back repeatedly to its original shape when pressure is removed. Changes in pressure alter the electrical resistance in silicon. (See *S&TR*, April 2006, pp. 4–9.)

Different MEMS contact sensors are designed to measure forces, pressures, accelerations, and gaps between components. “These sensors will enable us to take measurements that were never before possible,” says Kotovsky. Trebes notes that warheads are sometimes moved. “They are resilient to bumps and shakes,” he says. “However, if they are accidentally bumped, it would be useful to know what stress they received.” A MEMS-based sensor could measure that response.

The first of these sensors will be evaluated on joint test assemblies, weapons without nuclear components, which are used in tests aboard Department of Defense aircraft. Such testing ensures that weapons are compatible with the carriers that transport them. The MEMS sensors will report on the stresses that nonnuclear components experience during flight.

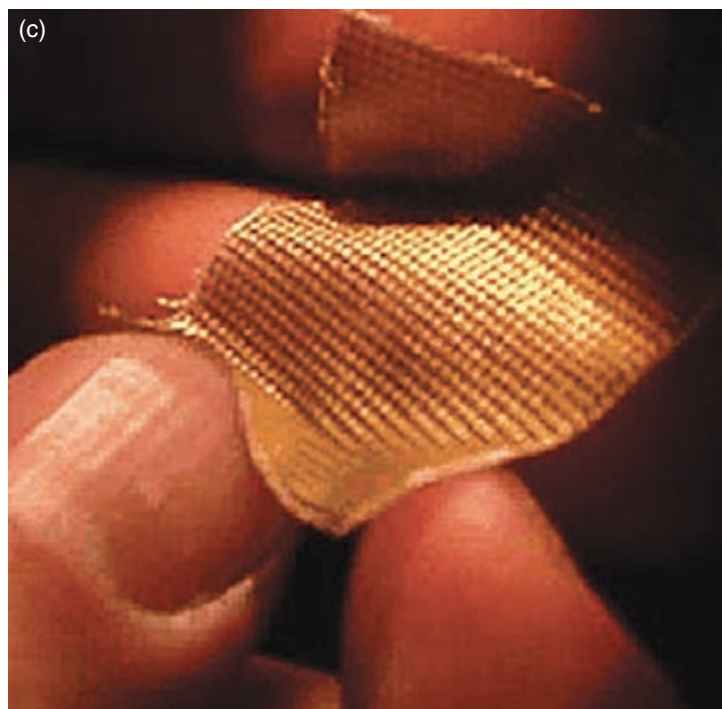
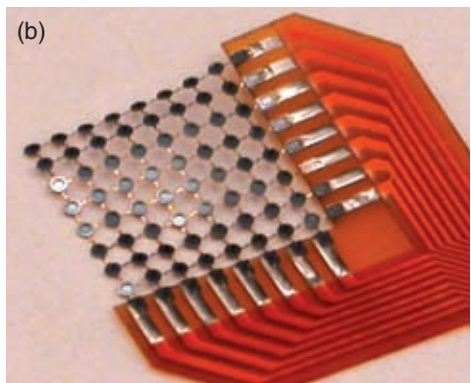
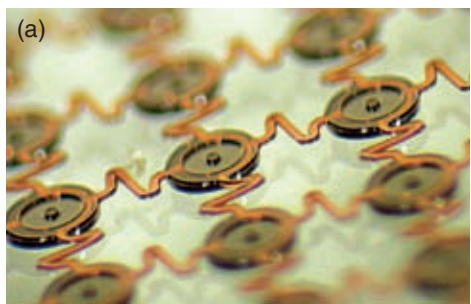
Sound Waves Tell the Truth

Livermore engineer Dave Chambers is studying acoustic techniques for detecting subtle structural changes in materials, including cracks, pits, voids, gaps, bends, and changes in density and elasticity. Acoustic waves are disturbances in mechanical vibrations in solids, liquids, or gases. Laboratory engineers have used acoustic techniques for years to nondestructively characterize materials. For example, says Chambers, some car mechanics can diagnose problems by listening carefully to the engine.

Chambers studied the response of components with different densities to the entire acoustic spectrum, ranging from human audio frequencies to ultrasound. He chose audio frequencies because these waves propagate through any kind of material.

The acoustic sensors use a fiber Bragg grating—an optical fiber embedded with a repeating pattern that allows only selected

(a) Individual sensors can be combined to form an array.
(b) One array has 64 units, shown here with electrical leads attached.
(c) A flexible array of 900 contact stress sensors can conform to any shape.



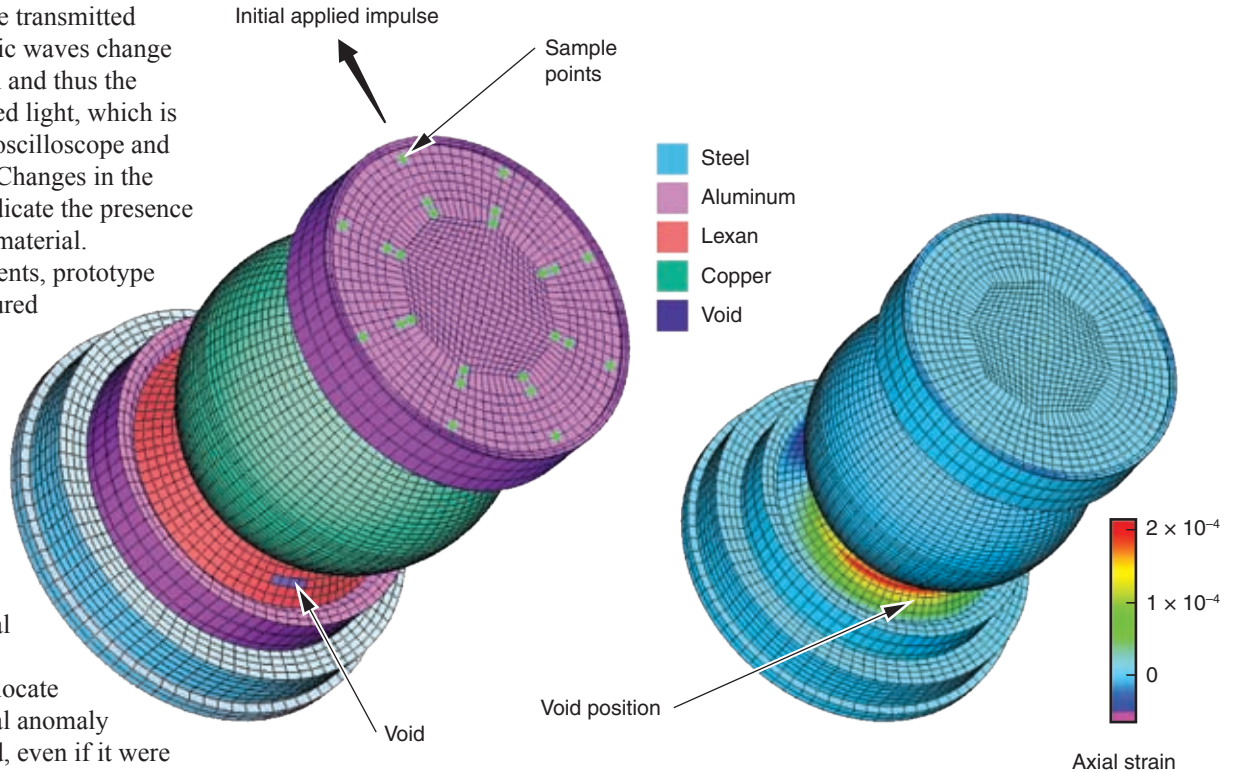
wavelengths of light to be transmitted through the fiber. Acoustic waves change the spacing of the pattern and thus the intensity of the transmitted light, which is recorded by a digitizing oscilloscope and archived on a computer. Changes in the acoustic response can indicate the presence of a crack or void in the material.

In laboratory experiments, prototype fiber-optic sensors measured the acoustic response at different points on a sample structure. Chambers is also using computer simulations to determine what engineers could learn from measurements supplied by a network of acoustic sensors. Initial results show that such a network could precisely locate the source of a vibrational anomaly caused by a crack or void, even if it were located deep within a part or assembly.

"Sometimes we only need to localize the problem," says Chambers. "The designer may be able to diagnose the problem just from knowing its location, especially if acoustic data are supplemented with measurements from another kind of sensor." Current simulations are modeling more complicated component geometries.

Leaving behind the Cold War

As costs continue to rise for maintaining the aging stockpile, a network of embedded sensors monitoring some or all of the nation's warheads seems to many experts a smart way to leave the Cold War legacy behind and introduce a new era of stockpile stewardship. Embedded sensors



In computer simulations of a hypothetical component made from different materials (left), a network of 18 acoustic sensors precisely locates the source of a flaw (void). Simulation results (right) indicate that axial strain increases near the void and potentially weakens the component.

would reduce or eliminate the transport and dismantlement of weapons, increase reliability, and enhance confidence in the enduring stockpile.

No one sensor is a complete solution by itself. But together, networks of embedded sensors could provide valuable information about the stockpile much earlier and at much less cost. In so doing, say Livermore weapons experts, the weapons complex and the stockpile would be well on the road to transformation.

—Arnie Heller

Key Words: embedded sensors, Fourier transform infrared (FTIR) spectroscopy, hydrogen getter, joint test assemblies, microelectromechanical systems (MEMS), Moscow Treaty on Strategic Offensive Reductions, nuclear stockpile, Raman spectroscopy, stockpile stewardship.

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Simulating the Biomolecular Structure of Nanometer-Size Particles

HUMAN disease caused by pathogens such as viruses and bacteria often results in infection. Infectious diseases may, in turn, affect human proteins and alter cellular function. Although researchers are still learning how those changes occur, the pharmaceutical industry often develops drugs to treat diseases by observing cell behavior. Nearly 60 percent of current drug molecules target proteins on the surface of cell membranes and partition the membrane's intracellular components from its extracellular environment.

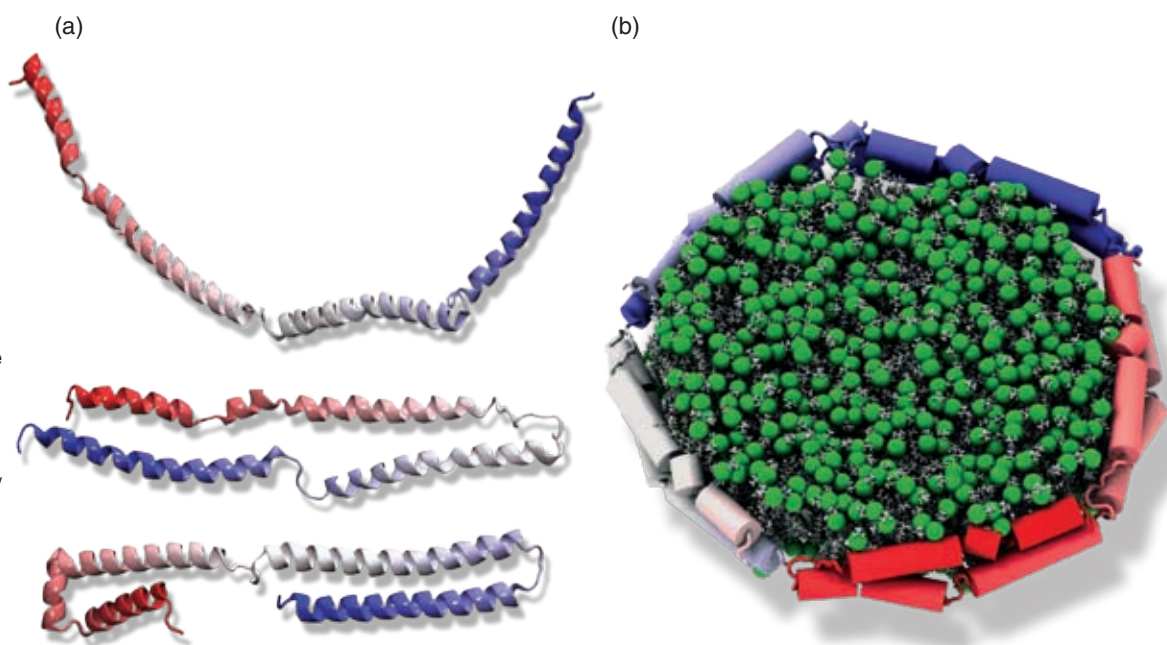
Membrane proteins are involved in an array of cellular processes required for organisms to survive, including energy production, communication between cells, and drug interactions. "Membrane proteins are the first responders or mediators for what passes through every cell in our body," says Livermore chemist Paul Hoeprich, who works in the Chemistry, Materials, Earth, and Life Sciences (CMELS) Directorate. "They connect the outside world to the inside cellular world."

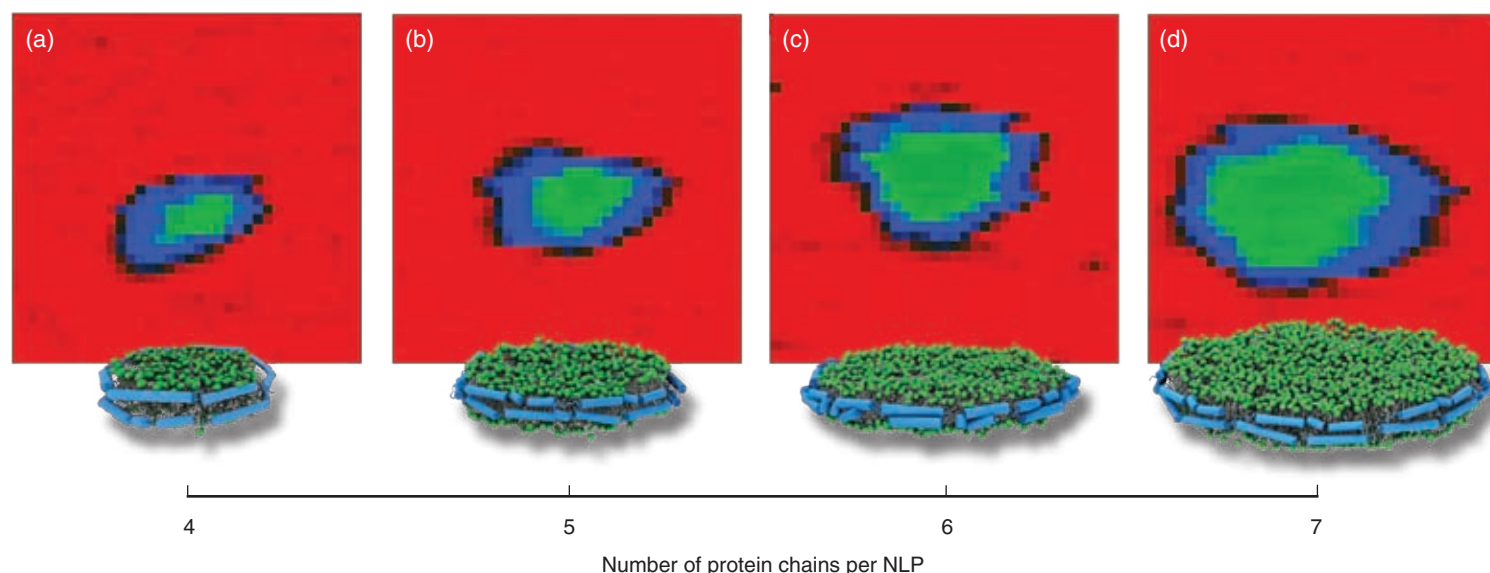
Membrane proteins are exceptionally difficult to study partly because they are insoluble and tend to aggregate or precipitate when removed from their natural environment. "A change in

environment will alter the structure of a membrane protein to such an extent that it becomes nonfunctioning," says computational chemist Richard Law, also in the CMELS Directorate. "In addition, these proteins are hydrophobic. To hide from water, they stick together and form a 'blob,' making it impossible to figure out how they function."

Because membrane proteins are insoluble, their structures cannot be easily mapped by x-ray crystallography, a technique commonly used to examine protein structures. Of the more than 45,000 protein structures known today, less than 1 percent are membrane proteins. To capture these proteins, scientists are constructing nanolipoprotein particles (NLPs) in the laboratory and using them as surrogates for cell membranes. NLPs are similar to the high- and low-density lipoprotein particles in the bloodstream—the "good" and "bad" cholesterol that moves fats and lipids through our bloodstream—and they mimic the membrane protein's natural cellular environment. Because NLPs are smaller and more stable in aqueous environments than the hydrophobic cell membranes, they offer an excellent platform for studying the structure and function of membrane proteins.

(a) Computer simulations show chains of the apolipoprotein E4-22K, where colors denote numbering from one end of a molecule (blue) to the other (red).
 (b) When chains link together around a group of lipids (green), they form a nanolipoprotein particle (NLP). Here, red, white, and blue denote individual folded proteins. An animated NLP is available online at www.llnl.gov/str/JulAug08/videos/nanolipoprotein.swf.





Atomic force microscopy images show that the number of protein chains surrounding a lipid determines the size of an NLP. Research indicates that NLPs occur in four sizes: (a) 14.5, (b) 19.0, (c) 23.5, and (d) 28.0 nanometers in diameter. (Micrographs taken by Craig Blanchette.)

A “Grand” Visualization

With funding from Livermore’s Laboratory Directed Research and Development (LDRD) Program, Hoeprich and Law are combining their expertise in experimental and computational science to model the structure of NLPs at the nanometer scale and examine protein behavior in detail. Law’s simulation effort is one of 17 projects selected for Livermore’s second annual Computing Grand Challenge Program. Each year, the Grand Challenge Program allocates time on Livermore’s high-performance computers to projects that are vital to the Laboratory’s missions, allowing researchers to simulate processes ranging from earthquakes to plutonium decay.

“Our ultimate goal is to analyze the structure and function of membrane proteins,” says Law. “First, we must understand the structure of a nanolipoprotein particle, which we will use to capture the membrane proteins involved in host–pathogen interactions.” Law’s simulations allow Hoeprich’s team to characterize the biomolecular structure of a protein called apolipoprotein and examine how it combines with lipids to create NLPs. Results from these simulations will also be used to design laboratory experiments with the Linac Coherent Light Source at the Stanford Linear Accelerator Center. (See the box on p. 22.)

High-Tech Tools

The NLP simulations were based on data acquired in laboratory experiments. Using high-resolution techniques such as atomic force microscopy, ion mobility spectroscopy, and electron

microscopy, Hoeprich and his team imaged thousands of the NLPs they assembled in the laboratory. In analyzing data from past experiments, they found that stable NLPs exist in four sizes—at 14.5, 19.0, 23.5, and 28.0 nanometers in diameter. Prior to this finding, researchers did not realize that NLPs could be quantized and would follow rules more closely associated with physics and physical chemistry. According to Hoeprich, the different imaging methods gave remarkably similar results about NLP structure, which provided a starting point for the simulations.

For the Grand Challenge project, Law developed calculations to run on the Thunder and Zeus supercomputers, two of the Laboratory’s Linux clusters. Using experimental data from Hoeprich’s team, Law modeled the structure of an apolipoprotein called E4-22K. He then simulated E4-22K apolipoproteins wrapping around a group of lipids to form the NLPs created in the laboratory.

Each NLP contains millions of atoms. Because atoms move so quickly, Thunder must take “snapshots” of a simulated NLP about every 2 femtoseconds (2 quadrillionths of a second, or 2×10^{-15} seconds) to accurately capture each atom’s position. After a few weeks of computer calculations, Thunder produced millions of snapshots, which were then combined to form continuous simulations, each 20 to 100 nanoseconds long.

Law’s high-resolution models corroborated the experimental results that E4-22K NLP structures occur in four distinct sizes. In addition, the simulations indicated that a particle’s size is related to the number of apolipoproteins surrounding the lipids. With E4-22K, four to seven protein chains surround the lipids.

The Linac Coherent Light Source

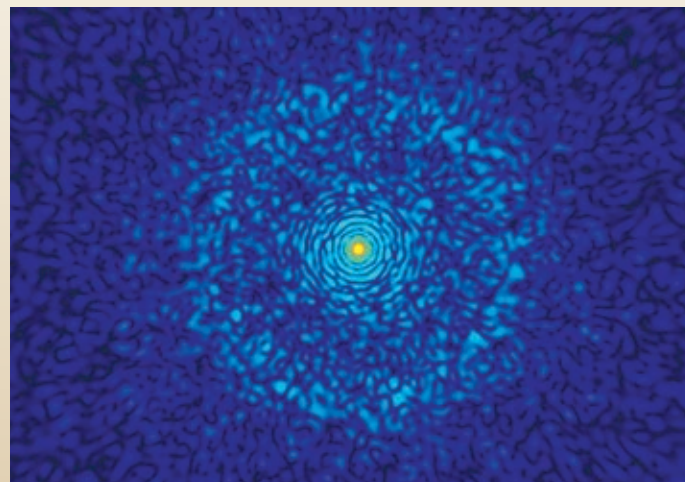
Although their methods are somewhat different, Livermore scientists Richard Law and Brian Bennion share a common “grand challenge” goal—to determine the structure and function of nanolipoprotein particles (NLPs) and membrane proteins. Using data from Law’s simulations, Bennion is modeling NLPs in very low-pressure environments to predict the behavior of a particle exposed to the x-ray beam of the Linac Coherent Light Source (LCLS).

LCLS is under construction at the Stanford Linear Accelerator Center and will come online in 2009. In the meantime, Bennion’s simulations are helping scientists plan for future LCLS experiments. His first set of simulations illustrates how the vacuum conditions required for the LCLS beam might influence the movement of NLP atoms. This information will be incorporated into a second set of simulations to determine how the vacuum conditions might affect NLP components such as water, proteins, and lipids.

In the LCLS experiments, an injector machine will spray tiny droplets of water mixed with NLPs through the vacuum chamber to the machine’s interaction region. Ideally, each water droplet will contain only one NLP. Inside the vacuum, an x-ray beam will strike the NLP–water droplet, and a camera will record the diffraction pattern as the x rays interact with the atoms of the NLP. By piecing together the recorded images, researchers can create a three-dimensional view of the particle.

Preliminary simulations indicate that if the shell of water surrounding an NLP is not uniformly thick, the diffraction pattern may be blurred because of uneven exposure to the x-ray beam. To determine if this prediction is accurate, Bennion plans to calculate thousands of diffraction patterns for the same NLP.

“It takes 12 hours of computing time to calculate a 1-picosecond molecular dynamics simulation of an NLP in vacuum conditions,” says Bennion. “We’d like to have at least 500 picoseconds total. That’s about a year’s worth of simulation time on a supercomputer running 24 hours a day.” With only about 25 picoseconds of data to date, the computer has a lot more work to do.



This snapshot from a Livermore simulation predicts the diffraction pattern that will occur when the Linac Coherent Light Source shoots an x-ray beam at a nanolipoprotein particle (NLP). Atomic bonds appear in the pattern’s outer rings. The yellow–red spot in the middle indicates where 95 percent of the beam traveled through the NLP to the machine’s beam stop.

“Law’s simulations have been extremely helpful because they allow us to visualize an NLP,” says Hoeprich. “Before this Grand Challenge project, no one had simulated the nanoparticles in so much detail.”

A Closer Look at Cell Behavior

Future simulations will focus on the process in which an intact membrane protein is implanted inside an NLP environment. “Now that we can determine the type and size of NLPs we’ve created,” says Law, “we can match them with the appropriate membrane proteins to examine the insertion process.” These simulations will help scientists determine whether the NLP environment is as similar to the membrane proteins’ natural environment as they believe it to be. This modeling effort will also advance research to determine how drugs interact with membrane protein receptors and the cells they affect—knowledge that is critical for developing potential treatments for diseases.

In addition, a better understanding of how membrane proteins assemble and function will help researchers evaluate cellular response to chemical and biological warfare agents. With such information, they can improve countermeasures and approaches for detecting and minimizing the threat of exposure to these agents. “Knowing a protein’s structure is important in understanding its function,” says Law, “and, in the case of disease, designing drugs to alter that behavior.”

—Kristen Light

Key Words: apolipoprotein E4-22K, Computing Grand Challenge Program, membrane protein, nanolipoprotein particle (NLP), protein structure, simulation, Thunder computer, Zeus computer.

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Antineutrino Detectors Improve Reactor Safeguards

WHAT has the ability to pass through anything, yet remain virtually undetected? No, it's not a superhero, but rather, stable elementary particles known as antineutrinos. These invisible particles seldom interact with matter, carry no electric charge, and have almost no mass. Yet, they are proving to be effective tools for global security. In a project funded by the National Nuclear Security Administration's Office of Nonproliferation Research and Development, scientists from Lawrence Livermore and Sandia national laboratories are developing antineutrino detectors to help the International Atomic Energy Agency (IAEA) safeguard fissile materials within nuclear reactors.

IAEA is the international organization responsible for monitoring nuclear facilities for nonproliferation purposes. For some of its assessments, the agency must rely on operator declaration. Antineutrino detectors could provide a more precise method to confirm that reactors are operating according to IAEA standards and that fissile materials are not being diverted for use in an undeclared nuclear weapons program. The Livermore–Sandia team has developed autonomous detectors that continuously and accurately monitor antineutrinos in real time throughout the one- to two-year fuel cycle of a standard pressurized water reactor.

Flashes of Light Reveal the Antineutrino

Reactor fuel rods contain the isotopes uranium-238 (^{238}U) and uranium-235 (^{235}U). Inside a reactor core, these isotopes absorb neutrons and undergo fission, producing antineutrinos with each decay. Some ^{238}U isotopes capture neutrons and decay into isotopes of plutonium-239 (^{239}Pu), which also fission and emit antineutrinos. However, the decay of ^{239}Pu produces substantially fewer antineutrinos than does the decay of ^{235}U within the energy range required for detection. Over the course of a reactor's fuel cycle, the antineutrino count rate drops as uranium content decreases and plutonium increases. In addition, the antineutrino count rate is proportional to the fission rate of the isotopes and thus is approximately proportional to the reactor's power. By monitoring this count rate, scientists can track both the thermal power and the fissile inventory of the reactor over time. Any deviation from what is considered "normal" would identify a potential problem.

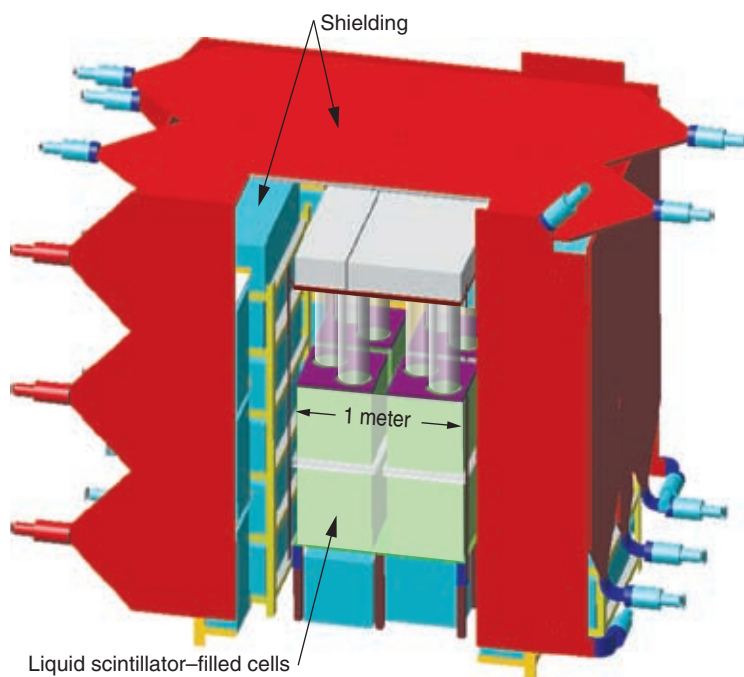
The Livermore–Sandia detectors are designed to measure inverse beta-decay interactions. When an antineutrino collides with a proton, it produces a positron and a neutron. The interactions of these two particles create the antineutrino signature—two relatively intense

flashes of light that occur so close in time to one another that they appear to be almost simultaneous. The bright two-step signature makes it easy to differentiate this interaction from those occurring in other processes, such as gamma-ray or ambient neutron interactions.

Testing, Testing . . . 1, 2, 3

The development team, led by physicists Adam Bernstein of Livermore and David Reyna of Sandia, is testing three prototype detectors at the San Onofre Nuclear Generating Station (SONGS) in San Clemente, California. The first detector, called SONGS1, has been operating there since 2004. (See *S&TR*, January/February 2006, pp. 21–23.)

SONGS1 uses a proton-rich liquid scintillator doped with gadolinium to induce the inverse beta-decay interactions. In this



SONGS1 is a liquid scintillator detector, one of three Livermore–Sandia prototypes being tested at the San Onofre Nuclear Generating Station (SONGS). Special shielding surrounds the liquid-filled cells inside the detector to protect them from background radiation and cosmic particles that could mimic the antineutrino signature.

design, an antineutrino from the reactor collides with a proton in the liquid, producing a positron and a neutron. Within a few nanoseconds, the positron, which carries away most of the antineutrino's energy, creates a flash of bluish scintillation light as it travels through the liquid and rapidly annihilates an electron. Gamma rays produced in this process induce further scintillation flashes. About 30 microseconds after the positron flash, the neutron that has traveled through the scintillator is captured by a nucleus of gadolinium. The neutron–gadolinium interaction also produces gamma rays, which immediately induce a second flash of light as they move through the liquid. Photomultiplier tubes detect these two bright light pulses, each only a few nanoseconds wide and separated by a few tens of microseconds.

For the prototype test, the team installed SONGS1 about 10 meters underground at a 25-meter standoff from the reactor core in an area known as the tendon gallery. The detector can operate continuously in this area without disrupting facility personnel or day-to-day operations. The tendon gallery also protects the detector from cosmic rays that could produce antineutrino events. At this location, about one in every 100,000 antineutrinos produced by the reactor passes through the detector. According to Bernstein, antineutrino interactions are fairly easy to detect, even though the particles themselves rarely interact with matter. Of the 10^{17} antineutrinos that pass through the detector each day, about 4,000 collide with protons. Of these 4,000, about 400 result in a detectable signature in this simple detector.

Although SONGS1 has been successful in its field test, the device has a few drawbacks. First, it is large and heavy, measuring 3 meters per side and weighing 25 tons, including a 20-ton water shield. Second, the liquid scintillator is flammable, toxic, and carcinogenic, so the unit must be transported as hazardous material.

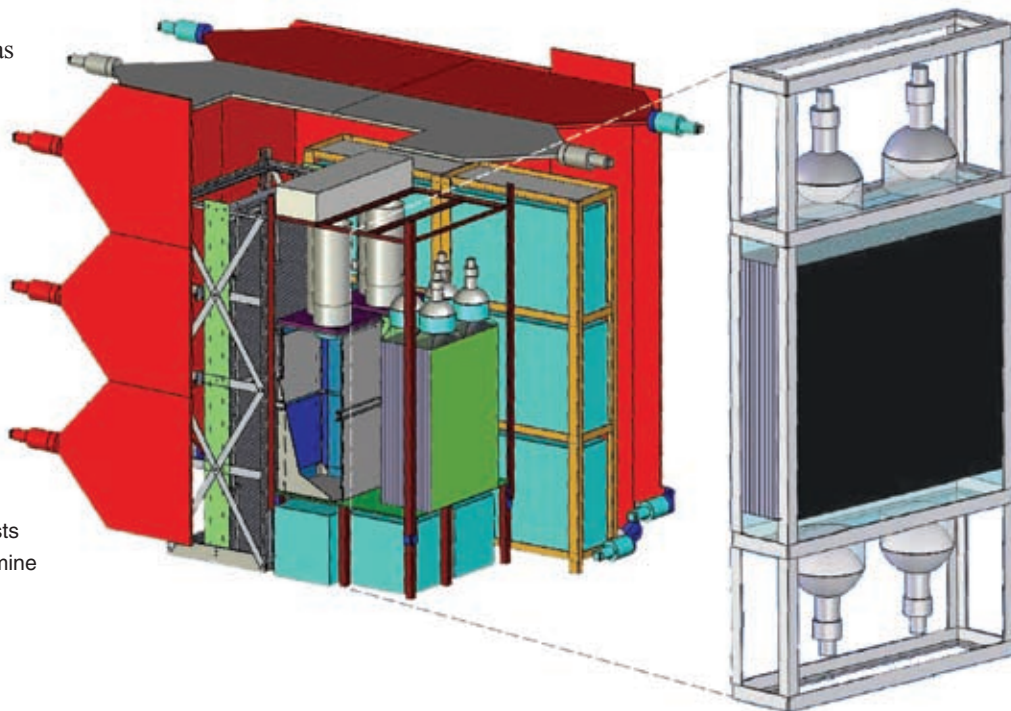
Deploying this type of detector worldwide would thus be difficult. As a result, the team has designed two other prototypes, SONGS2 and SONGS3, that operate with less hazardous materials. The team is also evaluating detection methods that could lead to a smaller device “footprint.”

SONGS2 uses a plastic scintillator instead of a liquid. Because gadolinium compounds degrade plastic's transparency, researchers mixed gadolinium into a

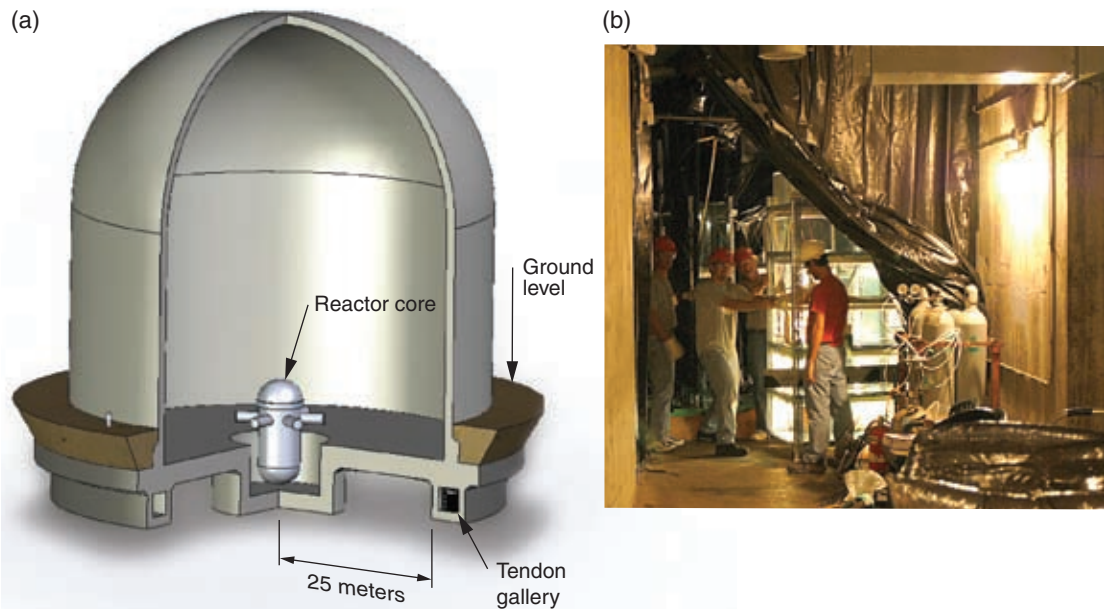
paint and applied a 1-millimeter-thick layer of the mixture onto 2-centimeter-thick plastic sheets. They then alternated the gadolinium-painted sheets with pieces of plastic scintillator. In this design, an incoming antineutrino collides with a proton in the plastic scintillator. The resulting positron creates the first flash of light, while the neutron travels randomly through the plastic until it is captured by a gadolinium nucleus in the paint. As in the liquid detector, the neutron–gadolinium reaction produces gamma rays, which easily escape the thin layer of paint to create a second flash of light in the plastic scintillator.

Instead of scintillation liquid or plastic, SONGS3 uses water mixed with gadolinium and measures Cerenkov light. Cerenkov light, predominantly ultraviolet but partially blue, is produced as charged particles move faster than the speed of light within the water. In this system, an antineutrino collides with a proton, which creates the positron and neutron. The first flash of Cerenkov light appears as the positron zips through the water. The neutron created during the antineutrino–proton collision is again captured by a gadolinium nucleus, producing the familiar gamma-ray cascade. These gamma rays in turn generate fast Compton-scattered electrons, which generate a second flash of Cerenkov light.

Although this water-based detector provides a measurable antineutrino signature, the interactions in water produce less light. According to Bernstein, “About 100 times fewer Cerenkov photons are generated compared with the amount of light produced in the liquid and plastic scintillators.” Despite this fainter signal, the detector does have its benefits. First, water is more benign than scintillation liquid. Second, the detector is impervious to high-energy neutron radiation caused by cosmic muons, which can mimic the antineutrino signature in scintillator detectors. Because all three



For the SONGS2 design, researchers replaced half of the liquid scintillator with a plastic scintillator (see inset). Results from field tests for the three prototypes will be compared to determine the effectiveness of each design.



(a) For the field tests, detector prototypes are housed in the tendon gallery at SONGS. (b) The tendon gallery is a ring-shaped area about 10 meters underground and 25 meters from the reactor core.

detectors are underground, they are somewhat protected from these cosmic particles. However, the two scintillation detectors still require special shielding. The team is conducting tests to determine the amount of shielding needed for the water-based detector.

The two new prototypes were installed in the same reactor as SONGS1 and tested during a reactor shutdown in December 2007. The team is evaluating data from all three detectors to compare their performance. In August 2008, the reactor will undergo required maintenance, and all three detectors must be removed. One or both of the newer detectors will be tested at a surface location to determine the potential for aboveground operation.

The team is also working with scientists from the University of Chicago to develop argon- and germanium-based systems that will detect antineutrinos through a process called coherent neutrino–nucleus scattering. In this process, an antineutrino collides with a nucleus of argon or germanium, which results in nuclear recoil. As the recoiling nucleus collides with its neighbors, it shakes loose a few electrons. The germanium-based detector, which is being developed at the University of Chicago, uses a sensitive transistor to extract and amplify the electrons. The argon detector uses a dual-phase detection process. In the first phase, the electron signal is produced in liquid argon. In the second phase, the signal is amplified in an argon gas blanket above the liquid to generate copious scintillator light, which is detected by photomultiplier tubes.

“The coherent scatter process has a much higher antineutrino interaction rate per volume of detection medium compared with detectors that rely on inverse beta decay,” says Bernstein. “This process has long been predicted but never observed. Detecting the coherent scatter signal with either approach would signify a major breakthrough.” Because detectors that use coherent scatter have a high probability of interaction per unit mass, they can also have a much smaller footprint, possibly as small as 1 cubic meter

with the necessary shielding. In April, the team installed the first germanium-based prototype detector at SONGS.

The Next Generation of Antineutrino Detection

The Laboratory’s antineutrino detection technology could offer the IAEA a more accurate, less time-consuming, and more cost-effective method for reactor assessments. Although more precise detectors have been developed to study the fundamental properties of neutrinos, they are often much larger and more expensive than the Livermore–Sandia designs. “Our detectors are robust and simple to operate and maintain, which allows for widespread deployment,” says Bernstein. The autonomous systems are also self-calibrating and require no maintenance for months at a time. Data about the detector, such as temperature, and the hourly antineutrino count rate are collected through a secure dial-up connection to Sandia and shared with teams at both sites.

Antineutrino detection research could also help in developing or improving devices to detect gamma rays and neutrons for other national security applications. According to Bernstein, “Antineutrino detector research is the perfect marriage between basic science and applications that are relevant to the Laboratory’s national security missions.” For a particle that has no electric charge and practically zero mass, the antineutrino may have a big future.

—Caryn Meissner

Key Words: antineutrino detector, Cerenkov light, coherent neutrino nucleus scattering, fissile material, International Atomic Energy Agency (IAEA), inverse beta decay, nuclear reactor safeguards, San Onofre Nuclear Generating Station (SONGS), scintillator.

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Continued from p. 2

semiconducting and metallic nanowires with diameters less than 20 nanometers. The research showed that in addition to trapping a single wire in a potential well, optoelectronic tweezers can trap arbitrarily large numbers of wires in a given area. The tweezers can also preserve the wires' position and orientation, which is critical for depositing metallic contacts on a nanoscale material.

Optoelectronic tweezers are already used to move micrometer-size polymer beads and living cells in fluid chambers. When low-intensity light is projected onto a photoconductive layer between two electrodes, it creates a nonuniform electric field, allowing particles to be manipulated by light-actuated virtual electrodes. When used in the nanowire tests, the optical power density of the optoelectronic tweezers was 100,000 times less than that of optical tweezers, and the nanoscale device moved individual wires four times faster.

The tweezers can be used to create vertically aligned nanowire arrays for solar energy conversion, thermoelectric cooling, and transistor applications. The team's research was featured on the cover of the February 2008 issue of *Nature Photonics*.

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Simulations predict ground motion of earthquakes

Livermore scientists are working to better understand how the ground will respond to the strong forces of an earthquake. In collaboration with the U.S. Geological Survey (USGS), the University of California at Berkeley, and URS Corporation, the researchers developed high-performance computing models that animate ground motion as waves moving outward, color-coded by intensity. The research appears in three papers published in the April 2008 edition of the *Bulletin of the Seismological*

Society of America on the 102nd anniversary of the 1906 San Francisco earthquake, which ruptured along the San Andreas Fault.

Shawn Larsen, a Livermore geophysicist and computer scientist, worked on two of the papers. In the first study, Larsen's team used the wave-propagation code E3D to estimate the ground motion that occurred in central and northern California during the 1906 earthquake and that might occur in hypothetical earthquakes along the San Andreas Fault. Team members ran simulations on three Livermore computing systems and the Earth Simulator supercomputer in Japan. The second study used observations of the 1989 Loma Prieta earthquake, which also ruptured along the San Andreas Fault, to validate models of the 1906 quake.

For the third study, a research team led by Livermore seismologist Arthur Rodgers used data from San Francisco Bay Area earthquakes to evaluate a three-dimensional geologic and seismic model created by USGS. Using observations from a network of seismic stations that record broadband data in this region, the team compared computed seismograms with observed recordings for 12 moderate quakes.

The three studies are part of Livermore's Computing Grand Challenge Program, which allocates computational resources to unclassified science projects that support the Laboratory's missions. A better understanding of ground motion during earthquakes will help policy makers develop regulations to enhance public safety and emergency response and will lead to improved engineering designs. These studies also support nonproliferation efforts to distinguish the seismic signals from earthquakes and explosions.

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Patents

Precision Tool Holder with Flexure-Adjustable, Three Degrees of Freedom for a Four-Axis Lathe

Matthew J. Bono, Robin L. Hibbard

U.S. Patent 7,337,700 B2

March 4, 2008

A precision tool holder positions a single-point cutting tool on a four-axis lathe so that the center of the radius of the tool nose is precisely aligned with the B axis of the machine tool. With this positioning, mesoscale components with complex three-dimensional shapes can be machined to submicrometer accuracy. Designed to fit on a commercial diamond-turning machine, the device uses three flexure-based mechanisms to adjust the cutting tool's position with submicrometer resolution. Two flexures move the tool laterally to align it with the B axis, and a third adjusts the tool's height. Micrometer adjusters can be driven manually for precise positioning. The tool holder simplifies the positioning process and thus substantially reduces setup time.

Sample Rotating Turntable Kit for Infrared Spectrometers

Joel Del Eckels, Gregory L. Klunder

U.S. Patent 7,339,169 B1

March 4, 2008

A turntable kit for infrared spectrometers can be used to rotate samples. The infrared spectrometer has a probe for analyzing the sample, and the rotatable cup, which holds the sample, is adapted to receive the probe. A reflectance standard is located in the sample cup. A sleeve placed near the cup is positioned to receive the probe. A rotator connected to a battery moves the sample cup.

Portable Compton Gamma-Ray Detection System

Mark S. Rowland, Mark E. Oldaker

U.S. Patent 7,339,172 B2

March 4, 2008

This Compton-scattered gamma-ray detector system has a gamma-ray spectrometer, an array of scintillators around the spectrometer, and a multichannel analyzer. A radiation shield surrounds the first scintillator in the annular array.

Filtered Back-Projection Algorithm for Compton Telescopes

Donald L. Gunter

U.S. Patent 7,345,283 B2

March 18, 2008

This method converts Compton camera data of incident-radiation flux on a celestial sphere into a two-dimensional image. The system detects coincident gamma-radiation flux arriving from various directions of a 2-sphere. Using a back-projection process, it maps these events onto the 2-sphere to produce a convolution integral. This integral is stereographically projected onto a 2-plane to produce a second convolution integral, which is deconvolved by the Fourier method. The resulting image is then projected onto the 2-sphere.

Electron Beam Diagnostic for Profiling High Power Beams

John W. Elmer, Todd A. Palmer, Alan T. Teruya

U.S. Patent 7,348,568 B2

March 25, 2008

This system can be used to characterize high-power electron beams at power levels up to 10 kilowatts. The system has a slit disk assembly with several radial slits. A conducting disk with the same number of radial slits is placed below the slit disk, and a Faraday cup is located below the conducting disk. A start-stop target is placed near the slit disk assembly. A heat sink prevents the system from overheating. A cooling system, using water, for example, can be integrated into the heat sink. The high-power beam is initially directed onto the start-stop target. Once it reaches full power, the beam rotates around the slit disk assembly. The Faraday cup assembly detects the beam when it enters the radial slits in either of the two disk assemblies. A trigger probe can also be integrated into the system to help determine the proper orientation of the beam during reconstruction. After the beam passes over each slit, it is rapidly translated back to the start-stop target to minimize the amount of time it is in contact with the slit disk. A computed tomography algorithm uses the recorded data to reconstruct the power density distribution of the beam.

Neutron Interrogation System Using High Gamma Ray Signature to Detect Contraband Special Nuclear Materials in Cargo

Dennis R. Slaughter, Bertram A. Pohl, Arden D. Dougan, Adam Bernstein, Stanley G. Prussin, Eric B. Norman

U.S. Patent 7,359,480 B2

April 15, 2008

A system for inspecting cargo uses neutrons to detect the presence of special nuclear material. Cargo is irradiated with neutrons. The neutrons produce fission products in special nuclear material, if it is present, which will then generate gamma rays. The detection of gamma rays thus indicates the presence of special nuclear material.

Awards

Jim Candy, chief scientist in Livermore's Engineering Directorate, received the **Helmholtz-Rayleigh Interdisciplinary Silver Medal** from the **Acoustical Society of America**. The award recognizes Candy's work on model-based signal- and image-processing techniques to improve the detection and measurement of underwater acoustics for applications in national security, materials science, and medicine.

The **Federal Laboratory Consortium for Technology Transfer (FLC)** honored two Laboratory teams for **excellence in technology transfer**. The first team, which developed a compact proton therapy system for treating cancer patients, includes **George Caporaso, Stephen Sampayan, Yu-Jiuan Chen, Genaro Mempin, Roger Werne, and James Tak** of Livermore; **Tod Stoltz** of the University of California (UC) at Davis; and **Dennis Matthews** of the UC Davis Cancer Center. The second team, which developed a portable neutron detector to help interdict illegal nuclear materials, includes **Mark Rowland, Dan Dietrich, Raymond Alvarez, Neal Snyderman, Manoj Prasad, Phillip Kerr, Doug Howard, Pedro Castro, Catherine Elizondo, and Ray Pierce** of Livermore; and **Tim Twomey and Daniel Upp** of AMETEK Inc.'s ORTEC Products Group. FLC is a nationwide program that helps link federal laboratory mission technologies and expertise with the marketplace.

Keith Carlisle in Engineering received an **Award of Excellence** from the **National Nuclear Security Administration's Defense Programs** "for excellence in planning, managing, and executing the modern turning center evaluation and selection process." Carlisle and other Livermore researchers are working with Los Alamos National Laboratory to design the next generation of shell machines for pit production at Los Alamos. Carlisle's design was selected over five others because it has a small footprint, takes advantage of modern machine technology, features a U.S. machine-tool supplier, and uses many commercially available parts, which helps reduce manufacturing costs.

The **American Physical Society (APS)** has selected five Laboratory researchers as **outstanding referees** of APS journals. The honorees are **Peter Beiersdorfer, Mau Hsiung Chen, and Ian Thompson** of the Physical Sciences Directorate; **Charles Cerjan** of the Weapons and Complex Integration Principal Directorate; and former Livermore researcher **William Hoover**. APS instituted the outstanding referee program this year to recognize scientists who have been exceptionally helpful in assessing manuscripts for

publication in APS journals. In its inaugural year, the program selected 534 referees for this lifetime award. In the future, APS will annually recognize about 130 of its 42,000 active referees.

Three Laboratory scientists are among 72 new **fellows** elected by **SPIE (International Society for Optical Engineering)** for significant scientific and technical contributions in the fields of optic, photonics, and imaging. Senior engineer **John S. Taylor**, who leads the Precision Systems and Manufacturing Group, was recognized for "precision engineering and specific achievements in optical engineering for reflective extreme ultraviolet optics and assembled systems." **Edward Moses**, principal associate director for the National Ignition Facility and Photon Science, was honored "for specific achievements in high-energy lasers." Livermore retiree **Alan Frank** was recognized for his achievements in high-speed photography and high-powered lasers.

Pam Hullinger, the Laboratory's chief veterinary officer, was inducted into the **Alameda County Women's Hall of Fame** for her work in science. Hullinger oversees the agricultural assay development work and foreign animal disease modeling program, both of which focus on preventing the introduction and mitigation effects of foreign animal diseases. She is the sixth current or former Laboratory employee to receive this honor.

Lisa Poyneer of Livermore's Engineering Technologies Division received the **2008 Zuhair A. Munir Award** from **UC Davis** for her dissertation, "Signal Processing for High-Precision Wavefront Control in Adaptive Optics." This award is Poyneer's second for her dissertation, which she completed in June 2007 under the mentorship of Bernard Levy in the UC Davis Department of Electrical and Computer Engineering.

Livermore scientist **Tom Isaacs** has been named to the **National Academy of Sciences' Nuclear and Radiation Studies Board**, which oversees studies on the safety, security, technical efficiency, and policy and societal issues arising from the application of nuclear and radiation-based technologies. In May, Isaacs began a yearlong leave to serve as a **consulting professor** at the **Stanford University Center for International Security and Cooperation**. The center's mission is to produce policy-relevant research on international security problems, train the next generation of security specialists, and influence policy making in international security. Isaacs heads the Laboratory's Office of Planning and Special Studies, which publishes *Science & Technology Review*.

The New Face of Industrial Partnerships

The Industrial Partnerships Office (IPO) is Lawrence Livermore's primary connection to the private sector and the conduit through which innovative Laboratory technologies make their way to commercial firms. Livermore has been licensing its technologies for many years, and among Department of Energy laboratories, it is a leader in royalty income. IPO's new director, Erik Stenehjem, and his staff plan to increase those numbers even more and have set a five-year goal of doubling the number of licenses with commercial companies. To that end, the Laboratory is simplifying its process of contracting with outside organizations to expedite the transfer of market-worthy inventions. To increase licensing, IPO is striving to make new Laboratory technologies more attractive to venture capitalists and the private sector. The staff has enlisted graduate students at business schools to write business plans that give potential investors the information they need on the Laboratory's inventions.

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Monitoring a Nuclear Weapon from the Inside

Monitoring the health of the nation's aging nuclear weapons stockpile has become a complicated and costly task. One of the most needed improvements is a cost-effective way to detect corrosion, cracks, or other changes without having to disassemble a weapon for inspection. A promising Livermore effort is developing tiny, rugged sensors that could be embedded in every nuclear weapon to provide the information currently obtained from disassembly. The sensors could make possible for the first time "persistent surveillance"—continuous monitoring of weapon components and practically instantaneous detection of anomalies. Many sensor designs use glass fibers measuring about 75 micrometers in diameter, smaller than the thickness of a human hair. Other designs are based on microelectromechanical systems (MEMS), which are fabricated from silicon with techniques similar to those used by the electronics industry.

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The Supernova Yardstick



Courtesy: NASA/ESA Hubble Space Telescope

High-resolution simulations are advancing understanding of Type Ia supernovae to help uncover the mysteries of dark energy.

Also in September/October

- Accelerator mass spectrometry emerges as a tool for assessing the pharmacokinetics and safety of new drugs.
- A painless on-and-off skin patch provides fast detection of exposure to biological pathogens, explosives, or radiation.
- A process for smoothing mask defects helps move extreme ultraviolet lithography one step closer to creating smaller, more powerful computer chips.

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